(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
30 August 2001 (30.08.2001)

PCT

(10) International Publication Number
WO 01/63244 A1

(51) International Patent Classification[7]: G01N 9/00, 33/48

(21) International Application Number: PCT/US01/05150

(22) International Filing Date: 16 February 2001 (16.02.2001)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
09/514,026 25 February 2000 (25.02.2000) US

(71) Applicant: AMERICAN HOME PRODUCTS CORPORATION [US/US]; Five Giralda Farms, Madison, NJ 07940-0874 (US).

(72) Inventors: CHEN, James, M.; 7 Sgt. David Stoddard Court, Bedminster, NJ 07921 (US). MOBILIO, Dominick; 35 Sneider Road, Warren, NJ 07059 (US). MOY, Franklin, J.; 37 Burch Street, Arlington, MA 02414 (US). PARRIS, Kevin, D.; 112 Woodbine Street, Auburndale, MA 02466 (US). POWERS, Robert; 3 Magnolia Drive, Westford, MA 01866 (US). BAO XU, Zhang; 40 Fieldston Circle, Tewksbury, MA 01876 (US).

(74) Agent: ARNOLD, Craig, J.: Amster, Rothstein & Ebenstein, 90 Park Avenue, New York, NY 10016 (US).

(81) Designated States *(national)*: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW.

(84) Designated States *(regional)*: ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG).

Published:
— *with international search report*
— *before the expiration of the time limit for amending the claims and to be republished in the event of receipt of amendments*

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

WO 01/63244 A1

(54) Title: SOLUTION AND CRYSTAL STRUCTURES OF MMP-13 ACTIVE SITE AND USES THEREOF

(57) Abstract: The present invention relates to the three dimensional structure of human collagenase 3 (MMP-13), as well as to (i) methods of using the MMP-13 structure to rationally design or identify compounds or molecules that inhibit or activate MMP-13 activity, and (ii) compounds identified using said methods.

Docket No. 2368/16

SOLUTION AND CRYSTAL STRUCTURES OF MMP-13 ACTIVE SITE AND USES THEREOF

Field of the Invention

The present invention relates to the three dimensional structure of human collagenase 3 (MMP-13), as well as to (i) methods of using the MMP-13 structure to rationally design or identify compounds or molecules that inhibit or activate MMP-13 activity, and (ii) compounds identified using said methods.

Background of the Invention

Human collagenase-3 (MMP-13) is a member of the matrix metalloproteinase (MMP) family which includes the collagenases, stromelysins and gelatinases. The MMPs are involved in the degradation of the extracellular matrix and are associated with normal tissue remodeling processes such as pregnancy, wound healing, and angiogenesis. MMP expression and activity is highly controlled because of the degradative nature of these enzymes, where an apparent loss in MMP regulation results in the pathological destruction of connective tissue and the ensuing disease state. Accordingly, MMPs are a highly active set of targets for the design of therapeutic agents for the disease areas of arthritis and oncology (for reviews, *see* Woessner, J. F., FASEB 1991; Ries, C., and Petrides, E., Biol. Chem. Hoppe-Seyler 1995; Browner, M. F., Perspect. Drug Discovery Des. 1995; Morphy, *et al.*, Curr. Med. Chem. 1995; and Zask, *et al.*, Curr. Pharm. Des. 1996).

MMP-13 was identified on the basis of differential expression in normal breast tissues and in breast carcinoma. In addition, its expression has been reported in squamous cell carcinomas of the larynx, head and neck, in HCS-2/8 human chondrosarcoma cells, during fetal ossification, and in articular cartilage of arthritic patients.

There have been a number of X-ray and NMR structures solved for the catalytic domain of MMPs complexed with a variety of inhibitors (*see e.g.*, Bode, *et al.*, EMBO J. 1994; Gooley, *et al.*, Nat. Struct. Biol. 1994; Lovejoy, *et al.*, Science 1994; Lovejoy, *et al.*, Ann. N. Y. Acad. Sci. 1994; Lovejoy, *et al.*,

Biochemistry 1994; Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994; Stams, *et al.*, Nat. Struct. Biol. 1994; Becker, *et al.*, Protein Sci. 1995; Gonnella, *et al.*, Proc. Natl. Acad. Sci. U.S.A. 1995; Van Doren, *et al.*, Protein Sci. 1995; Botos, *et al.*, Proc. Natl. Acad. Sci. USA 1996; Broutin, *et al.*, Acta Crystallogr., Sect. D: Biol. Crystallogr. 1996; Gooley, *et al.*, J. Biomol. NMR 1996; Betz, *et al.*, Eur. J. Biochem. 1997; Gonnella, *et al.*, Bioorg. Med. Chem. 1997; and Moy, *et al.*, Biochemistry 1998). There is a close similarity in the overall three-dimensional fold for these proteins consistent with the relatively high sequence homology (> 40%). Despite this similarity in the MMP structures, there is a distinct substrate specificity between these enzymes indicative of specific biological roles for the various MMPs and a corresponding association with unique disease processes. One example of this potential specificity is the over-expression of MMP-13 in breast carcinoma and MMP-1 in papillary carcinomas. Therefore, the current paradigm in the development of MMP inhibitors is to design specificity into the structures of the small molecule instead of developing a broad spectrum MMP inhibitor (Birkedal-Hansen, *et al.*, Crit. Rev. Oral Biol. Med. 1993; and Rockwell, *et al.*, J. Am. Chem. Soc. 1996). The rationale behind this approach is that an inhibitor specific for the MMP uniquely associated with a disease process may potentially minimize toxic side effects. Therefore, extensive structural information for the various MMPs is critical for a structure-based approach in designing inhibitor selectivity (Birkedal-Hansen, *et al.*, Crit. Rev. Oral Biol. Med. 1993; Rockwell, *et al.*, J. Am. Chem. Soc. 1996; Ghose, *et al.*, J. Am. Chem. Soc. 1995; Hajduk, *et al.*, J. Am. Chem. Soc. 1997; and Olejniczak, *et al.*, J. Am. Chem. Soc. 1997).

This concept has been facilitated by the extensive structural data available for the MMPs where a significant difference in the size and shape of the S1' pocket has been observed (Moy, *et al.*, Biochemistry 1998; Bode, *et al.*, EMBO J. 1994; Gooley, *et al.*, Nat. Struct. Biol. 1994; Lovejoy, *et al.*, Ann. N.Y. Acad. Sci. 1994; Lovejoy, *et al.*, Biochemistry 1994; Lovejoy, *et al.*, Science 1994; Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994; Stams, *et al.*, Nat. Struct. Biol. 1994; Becker, *et al.*, Protein Sci. 1995; Gonnella, *et al.*, Proc. Natl.

Acad. Sci. U.S.A. 1995; Van Doren, *et al.*, Protein Sci. 1995; Botos, *et al.*, Proc. Natl. Acad. Sci. U.S.A. 1996; Broutin, *et al.*, Acta Crystallogr., Sect. D: Biol. Crystallogr. 1996; Gooley, *et al.*, J. Biomol. NMR 1996; Betz, *et al.*, Eur. J. Biochem. 1997; and Gonnella, *et al.*, Bioorg. Med. Chem. 1997). This structural difference across the MMP family provides an obvious approach for designing specificity into potent MMP inhibitors by designing compounds that appropriately fill the available space in the S1' pocket while taking advantage of sequence differences. A number of examples have been previously reported using this approach where some selectivity between MMPs has been achieved by incorporating a biphenyl into the S1' pocket (*see e.g.*, Hajduk, *et al.*, J. Am. Chem. Soc. 1997; and Olejniczak, *et al.*, J. Am. Chem. Soc. 1997).

The inventors have determined both the solution and crystal structures of MMP-13, and, using rational drug design methods, have designed a novel, potent inhibitor that is highly selective for MMP-13.

Summary of the Invention

The present invention relates to the three dimensional structure of human collagenase 3 (MMP-13), and more specifically, to the crystal and solution structures of MMP-13 complexed with the inhibitor N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-methyl-benzamide (hereinafter referred to as "Compound A"), as determined using crystallography, spectroscopy and various computer modeling techniques. Particularly, the invention is directed to an MMP-13 active site comprised of the three dimensional structures of various binding pockets located both to the right (S1', S2', S3') and left (S1, S2, S3) of the catalytic zinc of MMP-13, and most particularly is directed to the three dimensional structure of an MMP-13 active site comprising the catalytic zinc and the S1' binding pocket, which is critical to the design and selection of inhibitors with increased potency and specificity for MMP-13, or conversely, for the design and selection of inhibitors of matrix metalloproteinases that are specific against MMP-13.

Accordingly, the present invention discloses a solution comprising a biologically active catalytic fragment of human collagenase-3 (MMP-13) complexed with Compound A, as well as a crystallized catalytic fragment of MMP-13 complexed with Compound A. The three dimensional structure of the catalytic fragment of MMP-13 is provided by the relative atomic structural coordinates of Figure 4, as obtained from spectroscopy data, and Figure 5, as obtained from crystallography data. Also provided is an active site of MMP-13, characterized by a catalytic zinc, a beta strand, a Ca^{2+} binding loop, an alpha helix and a random coil region, wherein the beta strand of said active site preferably comprises residues N14, L15, T16, Y17, R18, I19, and V20 according to Figure 1, the Ca^{2+} binding loop comprises residues F75, D76, G77, P78, and S79 according to Figure 1, the alpha helix comprises residues N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, and H123 according to Figure 1, and the random coil region comprises residues P139, I140, and Y141 according to Figure 1. Said active site is further characterized by a three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, ± a root mean square deviation from the catalytic zinc and conserved backbone atoms of said amino acids of not more than 1.5Å.

In an alternate embodiment of the invention, an active site of MMP-13 is characterized by a three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, ± a root mean square deviation from the catalytic zinc and conserved backbone atoms of said amino acids of not more than 1.5Å.

The solution or crystal structural coordinates of MMP-13 or portions thereof as provided by this invention may be stored in a

activator, and (ii) synthesizing or obtaining said potential inhibitor or activator. In this case, the potential inhibitor or activator is designed to incorporate chemical or steric features favorable for association with an active site of the desired matrix metalloproteinase(s) and unfavorable for association with an MMP-13 active site, preferably where said active site comprises the MMP-13 S1' pocket. The inhibitor or activator may be selected by screening an appropriate database, may designed *de novo* by analyzing the steric configurations and charge potentials of empty MMP-13/matrix metalloproteinase active sites in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors or activators to MMP-13 or other collagenases in order to create "hybrid" activators or inhibitors.

Also provided by the present invention are the inhibitors and activators designed or selected using the methods disclosed herein.

Brief Description of the Figures

Figure 1 depicts the amino acid sequence encoding the catalytic fragment of human MMP-13.

Figure 2 depicts the sequence based alignment between (A) MMP-13 and MMP-8 and (B) MMP-13 and MMP-1 used for the MMP-13 homology model.

Figure 3 is an illustration of the sulfonamide derivative of the hydroxamic inhibitor N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-methyl-benzamide (Compound A), with the corresponding proton labels.

Figure 4 lists the atomic structure coordinates for the restrained minimized mean structure of MMP-13 complexed with Compound A as derived by NMR spectroscopy. "Atom type" refers to the atom whose coordinates are being measured. "Residue" refers to the type of residue of which each measured atom is a part - i.e., amino acid, cofactor, ligand or solvent. The "x, y and z" coordinates indicate the Cartesian coordinates of each measured atom's location

three dimensional structure of MMP-13 as disclosed herein, and the three dimensional structure of the unknown molecule or molecular complex conformed to the known MMP-13 structure using standard techniques such as molecular replacement analysis, 2D, 3D and 4D isotope filtering, editing and triple resonance NMR techniques, and computer homology modeling. Alternatively, a three dimensional model of the unknown molecule may be generated by generating a sequence alignment between MMP-13 and the unknown molecule, based on any or all of amino acid sequence identity, secondary structure elements or tertiary folds, and then generating by computer modeling a three dimensional structure for the molecule using the three dimensional structure of, and sequence alignment with, MMP-13.

The present invention further provides a method for identifying a potential inhibitor or activator of MMP-13, comprising the steps of using a three dimensional structure of MMP-13 as defined by the relative structural coordinates of amino acids encoding MMP-13 to design or select a potential inhibitor or activator, and synthesizing or obtaining said potential inhibitor or activator. The inhibitor or activator may be selected by screening an appropriate database, may designed *de novo* by analyzing the steric configurations and charge potentials of an empty MMP-13 active site in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors or activators to MMP-13 or other collagenases in order to create "hybrid" activators or inhibitors. The method of the present invention is preferably used to design or select inhibitors of MMP-13 activity.

Alternatively, the present invention provides a method for identifying a potential inhibitor or activator that is selective for one or more members of the matrix metalloproteinase family except MMP-13, comprising the steps of (i) using the three dimensional structures of MMP-13 and the desired target matrix metalloproteinase(s) as defined by the relative structural coordinates of amino acids encoding MMP-13 and the target matrix metalloproteinase(s) in order to design or select such a potential inhibitor or

Detailed Description of the Invention

As used herein, the following terms and phrases shall have the meanings set forth below:

"Compound A" is N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-methyl-benzamide, as shown in Figure 3. "Compound B" is the compound having the chemical structure shown in Figure 6. "Compound C" is 2-[Benzyl-(4-phenethyloxy-benzenesulfonyl)-amino]-N-hydroxy-3,5-dimethyl-benzamide, as shown in Figure 7. "Compound D" is 2-[Benzyl-(4-methoxy-benzenesulfonyl)-amino]-N-hydroxy-3,5-dimethyl-benzamide, also shown in Figure 7. "Compound E" is Benzofuran-2-carboxylic acid (2-{4-[benzyl-(2-hydroxycarbamoyl-4,6-dimethyl-phenyl)-sulfamoyl]-phenoxy}-ethyl)-amide, as shown in Figure 8A. "Compound F" is 2-(Benzyl-4-(3-phenyl-propoxy)-benzenesulfonyl]-amino)-N-hydroxy-3,5-dimethyl-benzamide.

Unless otherwise noted, "MMP-13" includes both human collagenase 3 as encoded by the amino acid sequence of Figure 1 (including conservative substitutions thereof), as well as "MMP-13 analogues", defined herein as proteins comprising an MMP-13 like active site as defined by the present invention, including, but not limited to, an active site characterized by a three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, ± a root mean square deviation from the catalytic zinc and conserved backbone atoms of said amino acids of not more than 1.5Å, or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å. Alternatively, an MMP-13 analogue of the present invention is a protein which comprises an MMP-13 like active site characterized by a catalytic zinc, a beta strand, a Ca^{2+} binding loop, an alpha helix and a random coil region, or, more particularly, comprising an active site characterized by a three dimensional structure comprising the relative structural coordinates of the catalytic zinc and of amino acid residues N14, L15, T16, Y17, R18, I19, V20,

(Å). All non-protein atoms (Compound A, zinc and calcium) are listed as HETATM instead of atoms using PDB conventions.

Figure 5 lists the atomic structure coordinates for MMP-13 as derived by X-ray diffraction of a crystallized MMP-13:Compound A complex. Figure headings are as noted above, except "Occ" indicates the occupancy factor, and "B" indicates the "B-value", which is a measure of how mobile the atom is in the atomic structure ($Å^2$). "MOL" indicates the segment identification used to uniquely identify each molecule in the crystal.

Figure 6 is an illustration of the Compound B inhibitor, with the corresponding proton labels.

Figure 7 is a design scheme dividing 2-[Benzyl-(4-phenethyloxy-benzenesulfonyl)-amino]-N-hydroxy-3,5-dimethyl-benzamide (hereinafter referred to as "Compound C") into two components corresponding to its potency component (2-[Benzyl-(4-methoxy-benzenesulfonyl)-amino]-N-hydroxy-3,5-dimethyl-benzamide, hereinafter referred to as "Compound D") and its selectivity component, thereby providing the basis for the design of a hybrid inhibitor with Compound B.

Figure 8A is a design scheme showing the flow from Compound B and Compound C to the hybrid inhibitor benzofuran-2-carboxylic acid (2-{4-[benzyl-(2-hydroxycarbamoyl-4,6-dimethyl-phenyl)-sulfamoyl]-phenoxy}-ethyl)-amide (hereinafter referred to as "Compound E"). Figure 8B illustrates an expanded view of the NMR MMP-13:Compound B complex overlayed with the MMP-13:Compound D model, demonstrating the approach to forming the hybrid inhibitor Compound E. The MMP-13 active site is shown as a grid surface with Compound B and Compound D shown as liquorice bonds. The view is looking at the S1' pocket.

"Root mean square deviation" is the square root of the arithmetic mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from the structural coordinates described herein.

It will be obvious to the skilled practitioner that the numbering of the amino acid residues in the various isoforms of MMP-13 or in MMP-13 analogues covered by the present invention may be different than that set forth herein, or may contain certain conservative amino acid substitutions that yield the same three dimensional structures as those defined by Figures 4 or 5 herein. Corresponding amino acids and conservative substitutions in other isoforms or analogues are easily identified by visual inspection of the relevant amino acid sequences or by using commercially available homology software programs. "Conservative substitutions" are those amino acid substitutions which are functionally equivalent to the substituted amino acid residue, either by way of having similar polarity, steric arrangement, or by belonging to the same class as the substituted residue (e.g., hydrophobic, acidic or basic), and includes substitutions having an inconsequential effect on the three dimensional structure of MMP-13 with respect to the use of said structure for the identification and design of MMP-13 activators or inhibitors, for molecular replacement analyses and/or for homology modeling.

An "active site" refers to a region of a molecule or molecular complex that, as a result of its shape and charge potential, favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug). As such, the active site may include both the actual site of substrate cleavage or collagenase activity, as well as certain or all binding sites or pockets adjacent to the site of substrate cleavage that nonetheless may affect MMP-13 activity upon interaction or association with an agent, either by direct interference with the site of substrate cleavage or by indirectly affecting the steric conformation or charge potential of the MMP-13 molecule. The catalytic center of the MMP-13 molecule is characterized by a zinc atom chelated by H119, H123 and H129. MMP-13 binding sites or pockets located to the right of

F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to Figures 4 or 5, or more preferably, where said three dimensional structure further comprises the relative structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126, L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to Figures 4 or 5, or most preferably, where said three dimensional structure still further comprises the relative structural coordinates of F149 and P152 according to Figures 4 or 5, in each case, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms (N, Cα, C, and O) of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å).

Unless otherwise indicated, "protein" or "molecule" shall include a protein, protein domain, polypeptide or peptide.

"Structural coordinates" are the Cartesian coordinates corresponding to an atom's spatial relationship to other atoms in a molecule or molecular complex. Structural coordinates may be obtained using x-ray crystallography techniques or NMR techniques, or may be derived using molecular replacement analysis or homology modeling. Various software programs allow for the graphical representation of a set of structural coordinates to obtain a three dimensional representation of a molecule or molecular complex. The structural coordinates of the present invention may be modified from the original sets provided in Figures 4 or 5 by mathematical manipulation, such as by inversion or integer additions or subtractions. As such, it is recognized that the structural coordinates of the present invention are relative, and are in no way specifically limited by the actual x, y, z coordinates of Figures 4 and 5. Further, it is recognized that the structural coordinates taken from Figure 5 may be from either molecule of MMP-13 catalytic fragment in the MMP-13:Compound A crystal (i.e., from A-13 or B-13).

An "agent" shall include a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug.

Also provided by the present invention is a crystallized catalytic fragment of MMP-13 complexed with Compound A. The crystal of the present invention effectively diffracts X-rays for the determination of the structural coordinates of the MMP-13:Compound A complex, and is characterized as being in orthorhombic form with space group P21212, and having unit cell parameters of a=108.3Å, b=79.8Å, and c=36.1Å. Further, the crystal complex of the present invention consists of two molecules of MMP-13:Compound A complex in the asymmetric crystal unit.

In a preferred embodiment, the MMP-13 of the crystal complex of the present invention comprises the amino acid residues of Figure 1 (or conservative substitutions thereof), and is characterized by a secondary structure comprising three alpha helices and a mixed parallel and anti-parallel beta sheet comprising five beta strands, configured in the order β_I, α_A, β_{II}, β_{III}, β_{IV}, β_V, α_B, and α_C. Further, the three alpha helices preferably correspond to residues 28-44 (α_A), 112-123 (α_B) and 153-163 (α_C) of Figure 1, and the five beta strands correspond to residues 83-86 (β_I), 95-100 (β_{II}), 59-66 (β_{III}), 14-20 (β_{IV}), and 49-53 (β_V) of Figure 1, respectively.

The protein used in the crystal or crystal complex of the present invention includes MMP-13, as well as MMP-13 analogues, where said protein comprises an active site characterized by the three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 (or conservative substitutions thereof) according to the crystal coordinates of Figure 5, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å, or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å.

Alternatively, a protein used in the crystal or crystal complex of the present invention comprises an active site characterized by a catalytic zinc, a beta strand (comprising amino acid residues N14, L15, T16, Y17, R18, I19, and V20 or conservative substitutions thereof), a Ca^{2+} binding loop (comprising amino acid residues F75, D76, G77, P78, and S79 or conservative substitutions

the catalytic zinc include S1', S2' and S3'. Binding sites or pockets to the left of the catalytic zinc include S1, S2 and S3.

The present invention relates to the three dimensional structure of human collagenase 3 (MMP-13) or an MMP-13 analogue, and more specifically, to the crystal and solution structures of MMP-13 complexed with an inhibitor, referred to herein as "Compound A", as determined using crystallography, spectroscopy and various computer modeling techniques. The three dimensional solution and crystal structures of the MMP-13:Compound A complex (as disclosed herein at Figures 4 or 5, respectively) and the uncomplexed MMP-13 catalytic fragment (which may be computationally derived from the structural coordinates of Figures 4 or 5) are useful for a number of applications, including, but not limited to, the visualization, identification and characterization of MMP-13 active sites, including the MMP-13 catalytic zinc chelated by H119, H123 and H129, as well as the various MMP-13 binding pockets adjacent to the catalytic zinc of the MMP-13 molecule. The active site structures may then be used to predict the orientation and binding affinity of a designed or selected activator or inhibitor of the MMP-13 protein. Accordingly, the invention is particularly directed to the three dimensional structure of an MMP-13 active site, including but not limited to the S1', S2', S3', S1, S2 and/or S3 binding pockets, taken separately or together with the catalytic zinc of the MMP-13 molecule.

The present invention provides a solution comprising a biologically active catalytic fragment of human collagenase-3 (MMP-13) complexed with Compound A. In a particular embodiment, the catalytic fragment of MMP-13 comprises the amino acid residues of Figure 1, or conservative substitutions thereof. Preferably, the solution provided for herein comprises MMP-13 complexed with Compound A in a 1:1 molar ratio, and more preferably comprises 1 mM MMP-13 in an equimolar complex with Compound A, in a buffer comprising 10mM deuterated Tris-Base, 100mM NaCl, 5mM $CaCl_2$, 0.1mM $ZnCl_2$, 2mM NaN_3, and 10 mM deuterated DTT in either 90% H_2O/10% D_2O or 100% D_2O, at a preferred pH of 6.5. The concentration of

MMP-13:Compound A in the solution should be high enough to yield a good signal-to-noise ratio in the NMR spectrum, but not so high as to result in precipitation or aggregation of the protein. Further, the MMP-13 of the solution may be either ^{15}N enriched or $^{15}N,^{13}C$ enriched. As exemplified below, NMR spectra from the solution of the present invention are preferably obtained at a temperature of 35°C.

The secondary structure of the catalytic fragment used in the solution of the present invention comprises three alpha helices and a mixed parallel and anti-parallel beta sheet comprising five beta strands, configured in the order β_I, α_A, β_{II}, β_{III}, β_{IV}, β_V, α_B, and α_C. The three alpha helices correspond to residues 28-44 (α_A), 112-123 (α_B) and 153-163 (α_C) of Figure 1, and the five beta strands correspond to residues 83-86 (β_I), 95-100 (β_{II}), 59-66 (β_{III}), 14-20 (β_{IV}), and 49-53 (β_V) of Figure 1, respectively. While the solution of the present invention comprises MMP-13 in a 1:1 molar ratio with Compound A, it is understood that one of ordinary skill in the art may devise additional solutions using alternate inhibitors or ligands in the appropriate molar concentrations, thereby preventing the auto-degradation of MMP-13 and creating a solution of sufficient stability and concentration to obtain a usable NMR spectrum.

The protein used in the solution of the present invention includes MMP-13, as well as MMP-13 analogues, where said protein comprises an active site characterized by the three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 (or conservative substitutions thereof) according to the solution coordinates of Figure 4, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å, or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å. These residues comprise the residues most closely associated with Compound A in the MMP-13:Compound A complex, as determined from the observed NOEs between MMP-13 and Compound A (Table 1).

thereof), an alpha helix (comprising amino acid residues N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, and H123 or conservative substitutions thereof) and a random coil region (comprising amino acid residues P139, I140, and Y141 or conservative substitutions thereof), or, more particularly, characterized by a three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to Figure 5, or more preferably, where said three dimensional structure further comprises the relative structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126, L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to Figure 5 (incorporating an S1' pocket in the active site), or most preferably, where said three dimensional structure still further comprises the relative structural coordinates of F149 and P152 according to Figure 5 (further defining a hydrophobic area at the bottom of the S1' pocket), in each case, including conservative substitutions of the said amino acids and, in each case, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å).

Finally, in the most preferred embodiment, the protein used in the crystal of the present invention comprises the complete structural coordinates according to Figure 5, ± a root mean square deviation from the conserved backbone atoms of said amino acids (or conservative substitutions thereof) of not more than 1.5Å (or more preferably, not more than 1.0Å, and most preferably, not more than 0.5Å).

Molecular modeling methods known in the art may be used to identify an active site or binding pocket of the MMP-13 molecule, MMP-13 molecular complex, or an MMP-13 analogue. Specifically, the structural coordinates provided by the present invention may be used to characterize a

three dimensional model of the MMP-13 molecule, molecular complex or MMP-13 analogue. From such a model, putative active sites may be computationally visualized, identified and characterized based on the surface structure of the molecule, surface charge, steric arrangement, the presence of reactive amino acids, regions of hydrophobicity or hydrophilicity, etc. Such putative active sites may be further refined using chemical shift perturbations of spectra generated from various and distinct MMP-13 complexes, competitive and non-competitive inhibition experiments, and/or by the generation and characterization of MMP-13 mutants to identify critical residues or characteristics of the active site.

The identification of putative active sites of a molecule or molecular complex is of great importance, as most often the biological activity of a molecule or molecular complex results from the interaction between an agent and one or more active sites of the molecule or molecular complex. Accordingly, the active sites of a molecule or molecular complex are the best targets to use in the design or selection of activators or inhibitors that affect the activity of the molecule or molecular complex.

The present invention is directed to an active site of MMP-13 or an MMP-13 analogue, that, as a result of its shape, reactivity, charge potential, etc., favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibiotic or drug). As such, the active site of the present invention includes both the actual site of substrate cleavage or collagenase activity (the catalytic zinc chelated by H119, H123, and H129), as well as binding sites or pockets adjacent to the site of substrate cleavage (i.e., S1', S2', S3', S1, S2, and/or S3) that may nonetheless affect MMP-13 activity upon interaction or association with an agent, either by direct interference with the site of substrate cleavage or by indirectly affecting the steric conformation or charge potential of the MMP-13 molecule. Accordingly, the present invention is directed to an active site of the MMP-13 molecule characterized by a zinc atom chelated by H119, H123 and H129, and preferably the S1' binding pocket to the right of the catalytic zinc.

In an alternate embodiment, the active site of the present invention is characterized by the three dimensional structure comprising the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 (or conservative substitutions thereof) according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å, or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å.

Alternatively, the active site of the present invention is characterized by a catalytic zinc, a beta strand (comprising amino acid residues N14, L15, T16, Y17, R18, I19, and V20 or conservative substitutions thereof), a Ca^{2+} binding loop (comprising amino acid residues F75, D76, G77, P78, and S79 or conservative substitutions thereof), an alpha helix (comprising amino acid residues N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, and H123 or conservative substitutions thereof) and a random coil region (comprising amino acid residues P139, I140, and Y141 or conservative substitutions thereof), or, more particularly, is characterized by a three dimensional structure comprising the relative solution or crystal structural coordinates of the catalytic zinc and amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to Figures 4 or 5, respectively, or more preferably, where said three dimensional structure further comprises the relative solution or crystal structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126, L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to Figures 4 or 5, or most preferably, where said three dimensional structure still further comprises the relative solution or crystal structural coordinates of F149 and P152 according to Figures 4 or 5, in each case, including conservative substitutions of said amino acids, and in each case, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å

(or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å).

In order to use the structural coordinates generated for a crystal or solution structure of the present invention as set forth in Figures 4 and 5, respectively, it is often necessary to display the relevant coordinates as, or convert them to, a three dimensional shape or graphical representation, or to otherwise manipulate them. For example, a three dimensional representation of the structural coordinates is often used in rational drug design, molecular replacement analysis, homology modeling, and mutation analysis. This is typically accomplished using any of a wide variety of commercially available software programs capable of generating three dimensional graphical representations of molecules or portions thereof from a set of structural coordinates. Examples of said commercially available software programs include, without limitation, the following: GRID (Oxford University, Oxford, UK); MCSS (Molecular Simulations, San Diego, CA); AUTODOCK (Scripps Research Institute, La Jolla, CA); DOCK (University of California, San Francisco, CA); Flo99 (Thistlesoft, Morris Township, NJ); Ludi (Molecular Simulations, San Diego, CA); QUANTA (Molecular Simulations, San Diego, CA); Insight (Molecular Simulations, San Diego, CA); SYBYL (TRIPOS, Inc., St. Louis. MO); and LEAPFROG (TRIPOS, Inc., St. Louis, MO).

For storage, transfer and use with such programs, a machine, such as a computer, is provided for that produces a three dimensional representation of the MMP-13 molecule, a portion thereof (such as an active site or a binding site), a MMP-13 molecular complex, or an MMP-13 analogue. The machine of the present invention comprises a machine-readable data storage medium comprising a data storage material encoded with machine-readable data. Machine-readable storage media comprising data storage material include conventional computer hard drives, floppy disks, DAT tape, CD-ROM, and other magnetic, magneto-optical, optical, floptical and other media which may be adapted for use with a computer. The machine of the present invention also comprises a working memory for storing instructions for processing the

machine-readable data, as well as a central processing unit (CPU) coupled to the working memory and to the machine-readable data storage medium for the purpose of processing the machine-readable data into the desired three dimensional representation. Finally, the machine of the present invention further comprises a display connected to the CPU so that the three dimensional representation may be visualized by the user. Accordingly, when used with a machine programmed with instructions for using said data, *e.g.*, a computer loaded with one or more programs of the sort identified above, the machine provided for herein is capable of displaying a graphical three-dimensional representation of any of the molecules or molecular complexes, or portions of molecules of molecular complexes, described herein.

In one embodiment of the invention, the machine-readable data comprises the relative structural coordinates of the catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 according to Figures 4 or 5, in each case, including conservative substitutions thereof, and in each case, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, and most preferably, not more than 0.5Å), wherein said structural coordinates characterize an active site of MMP-13 or an MMP-13 analogue.

In an alternate preferred embodiment, the machine-readable data comprises the structural coordinates of the catalytic zinc and amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to Figures 4 or 5, in each case, including conservative substitutions thereof, and in each case, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, and most preferably, not more than 0.5Å). In an even more preferred embodiment, the machine-readable data further comprises the relative structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126,

L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to Figures 4 or 5, or most preferably, still further comprises the relative structural coordinates of F149 and P152 according to Figures 4 or 5, in each case, including conservative substitutions of said amino acids, and in each case, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å).

Finally, it is most preferred that the machine-readable data comprise the relative structural coordinates of all residues constituting the MMP-13 catalytic fragment according to Figures 4 or 5, in each case, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å. In each case, the noted embodiments comprise conservative substitutions of the noted residues resulting in same structural coordinates within the stated root mean square deviation.

The structural coordinates of the present invention permit the use of various molecular design and analysis techniques in order to (i) solve the three dimensional structures of related molecules, molecular complexes or MMP-13 analogues, and (ii) to design, select, and synthesize chemical agents capable of favorably associating or interacting with an active site of an MMP-13 molecule or MMP-13 analogue, wherein said chemical agents potentially act as activators or inhibitors of MMP-13 or of an MMP-13 analogue.

More specifically, the present invention provides a method for determining the molecular structure of a molecule or molecular complex whose structure is unknown, comprising the steps of obtaining crystals or a solution of the molecule or molecular complex whose structure is unknown, and then generating x-ray diffraction data from the crystallized molecule or molecular complex, and/or generating NMR data from the solution of the molecule or molecular complex. The x-ray diffraction data from the molecule or molecular complex whose structure is unknown is then compared to the x-ray diffraction data obtained from the MMP-13:Compound A crystal of the present invention.

Alternatively, the NMR data from the molecule or molecular structure whose structure is unknown is then compared with the NMR data obtained from the MMP-13:Compound A solution of the present invention. Then, molecular replacement analysis is used to conform the three dimensional structure determined from the MMP-13:Compound A crystal of solution of the present invention to the x-ray diffraction data from the unknown molecule or molecular complex, or, alternatively, 2D, 3D and 4D isotope filtering, editing and triple resonance NMR techniques are used to conform the three dimensional structure determined from the MMP-13:Compound A solution of the present invention to the NMR data from the solution molecule or molecular complex.

Molecular replacement analysis uses a molecule having a known structure as a starting point to model the structure of an unknown crystalline sample. This technique is based on the principle that two molecules which have similar structures, orientations and positions will diffract x-rays similarly. A corresponding approach to molecular replacement is applicable to modeling an unknown solution structure using NMR technology. The NMR spectra and resulting analysis of the NMR data for two similar structures will be essentially identical for regions of the proteins that are structurally conserved, where the NMR analysis consists of obtaining the NMR resonance assignments and the structural constraint assignments, which may contain hydrogen bond, distance, dihedral angle, coupling constant, chemical shift and dipolar coupling constant constraints. The observed differences in the NMR spectra of the two structures will highlight the differences between the two structures and identify the corresponding differences in the structural constraints. The structure determination process for the unknown structure is then based on modifying the NMR constraints from the known structure to be consistent with the observed spectral differences between the NMR spectra.

Accordingly, in one non-limiting embodiment of the invention, the resonance assignments for the MMP-13:Compound A complex provide the starting point for resonance assignments of MMP-13 in a new MMP-13:"unsolved agent" complex. Chemical shift perturbances in two dimensional

$^{15}N/^{1}H$ spectra can be observed and compared between the MMP-13:Compound A complex and the new MMP-13:agent complex. In this way, the affected residues may be correlated with the three dimensional structure of MMP-13 as provided by the relevant residues of Figure 4. This effectively identifies the region of the MMP-13:agent complex that has incurred a structural change relative to the MMP-13:Compound A complex. The ^{1}H, ^{15}N, ^{13}C and ^{13}CO NMR resonance assignments corresponding to both the sequential backbone and side-chain amino acid assignments of MMP-13 may then be obtained and the three dimensional structure of the new MMP-13:agent complex may be generated using standard 2D, 3D and 4D triple resonance NMR techniques and NMR assignment methodology, using the MMP-13:Compound A structure, resonance assignments and structural constraints as a reference. Various computer fitting analyses of the new agent with the three dimensional model of MMP-13 may be performed in order to generate an initial three dimensional model of the new agent complexed with MMP-13, and the resulting three dimensional model may be refined using standard experimental constraints and energy minimization techniques in order to position and orient the new agent in association with the three dimensional structure of MMP-13.

The present invention further provides that the structural coordinates of the present invention may be used with standard homology modeling techniques in order to determine the unknown three-dimensional structure of a molecule or molecular complex. Homology modeling involves constructing a model of an unknown structure using structural coordinates of one or more related protein molecules, molecular complexes or parts thereof (*i.e.*, active sites). Homology modeling may be conducted by fitting common or homologous portions of the protein whose three dimensional structure is to be solved to the three dimensional structure of homologous structural elements in the known molecule, specifically using the relevant (i.e., homologous) structural coordinates provided by Figures 4 and/or 5 herein. Homology may be determined using amino acid sequence identity, homologous secondary structure elements, and/or homologous tertiary folds. Homology modeling can

include rebuilding part or all of a three dimensional structure with replacement of amino acids (or other components) by those of the related structure to be solved.

Accordingly, a three dimensional structure for the unknown molecule or molecular complex may be generated using the three dimensional structure of the MMP-13:Compound A complex of the present invention, refined using a number of techniques well known in the art, and then used in the same fashion as the structural coordinates of the present invention, for instance, in applications involving molecular replacement analysis, homology modeling, and rational drug design.

Determination of the three dimensional structure of MMP-13 and its catalytic active site as disclosed herein is critical to the rational identification and/or design of therapeutic agents that may act as inhibitors or activators of MMP-13 enzymatic activity. Alternatively, using conventional drug assay techniques, the only way to identify such an agent is to screen thousands of test compounds, either in culture or by administration to suitable animal models in a laboratory setting, until an agent having the desired inhibitory or activating effect on a target compound is identified. Necessarily, such conventional screening methods are expensive, time consuming, and do not elucidate the method of action of the identified agent on the target compound.

However, advancing X-ray, spectroscopic and computer modeling technologies allow researchers to visualize the three dimensional structure of a targeted compound. Using such a three dimensional structure, researchers identify putative binding sites and then identify or design agents to interact with these binding sites. These agents are then screened for an activating or inhibitory effect upon the target molecule. In this manner, not only are the number of agents to be screened for the desired activity greatly reduced, but the mechanism of action on the target compound is better understood.

Accordingly, the present invention further provides a method for identifying a potential inhibitor or activator of MMP-13, comprising the steps of using a three dimensional structure of MMP-13 as defined by the relative

structural coordinates of amino acids encoding MMP-13 to design or select a potential inhibitor or activator, and synthesizing or obtaining said potential inhibitor or activator. The inhibitor or activator may be selected by screening an appropriate database, may designed *de novo* by analyzing the steric configurations and charge potentials of an empty MMP-13 active site in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors or activators to MMP-13 or other collagenases in order to create "hybrid" activators or inhibitors. The method of the present invention is preferably used to design or select inhibitors of MMP-13 activity.

An agent that interacts or associates with an active site of MMP-13 or an MMP-13 analogue may be identified by determining an active site of MMP-13 or of the MMP-13 analogue from a three dimensional model of the MMP-13 or MMP-13 analogue, and performing computer fitting analyses to identify an agent which interacts or associates with said active site. Computer fitting analyses utilize various computer software programs that evaluate the "fit" between the putative active site and the identified agent, by (a) generating a three dimensional model of the putative active site of a molecule or molecular complex using homology modeling or the atomic structural coordinates of the active site, and (b) determining the degree of association between the putative active site and the identified agent. The degree of association may be determined computationally by any number of commercially available software programs, or may be determined experimentally using standard binding assays.

Three dimensional models of the putative active site may be generated using any one of a number of methods known in the art, and include, but are not limited to, homology modeling as well as computer analysis of raw structural coordinate data generated using crystallographic or spectroscopy techniques. Computer programs used to generate such three dimensional models and/or perform the necessary fitting analyses include, but are not limited to: GRID (Oxford University, Oxford, UK), MCSS (Molecular Simulations, San Diego, CA), AUTODOCK (Scripps Research Institute, La Jolla,

CA), DOCK (University of California, San Francisco, CA), Flo99 (Thistlesoft, Morris Township, NJ), Ludi (Molecular Simulations, San Diego, CA), QUANTA (Molecular Simulations, San Diego, CA), Insight (Molecular Simulations, San Diego, CA), SYBYL (TRIPOS, Inc., St. Louis. MO) and LEAPFROG (TRIPOS, Inc., St. Louis, MO).

In a preferred method of the present invention, the identified active site of MMP-13 or the MMP-13 analogue comprises a catalytic zinc, a beta strand, a Ca^{2+} binding loop, an alpha helix and a random coil region. More preferably, the identified active site comprises a catalytic zinc, a beta strand comprising residues N14, L15, T16, Y17, R18, I19, and V20 according to Figure 1 (or conservative substitutions thereof), a Ca^{2+} binding loop comprising residues F75, D76, G77, P78, and S79 according to Figure 1 (or conservative substitutions thereof), an alpha helix comprising residues N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, and H123 according to Figure 1 (or conservative substitutions thereof), and a random coil region comprising residues P139, I140, and Y141 according to Figure 1 (or conservative substitutions thereof).

More specifically, the identified active site of the present method comprises the relative structural coordinates of the catalytic zinc and amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to Figures 4 or 5, in each case, including conservative substitutions of said amino acids, and in each case, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å). In an alternate preferred embodiment, the identified active site further comprises the relative structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126, L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to Figures 4 or 5, in each case, including conservative substitutions of said amino acids, and in each case,

± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å). In yet a third preferred embodiment, the identified active site of the present method further comprises the relative structural coordinates of amino acid residues F149 and P152 according to Figures 4 or 5, in each case, including conservative substitutions of said amino acids, and in each case, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å (or more preferably, not more than 1.0Å, or most preferably, not more than 0.5Å). Embodiments comprising conservative substitutions of the noted amino acids result in the same structural coordinates of the corresponding residues in Figures 4 or 5 within the stated root mean square deviation.

The effect of such an agent identified by computer fitting analyses on MMP-13 (or MMP-13 analogue) activity may be further evaluated computationally, or experimentally by contacting the identified agent with MMP-13 (or an MMP-13 analogue) and measuring the effect of the agent on the enzyme's activity. Depending upon the action of the agent on the active site of MMP-13, the agent may act either as an inhibitor or activator of MMP-13 activity. Standard enzymatic assays may be performed and the results analyzed to determine whether the agent is an inhibitor of MMP-13 activity (i.e., the agent may reduce or prevent binding affinity between MMP-13 and the relevant substrate, and thereby reduce the level or rate of MMP-13 activity compared to baseline), or an activator of MMP-13 activity (i.e., the agent may increase binding affinity between MMP-13 and the relevant substrate, and thereby increase the level or rate of MMP-13 activity compared to baseline). Further tests may be performed to evaluate the selectivity of the identified agent to MMP-13 with regard to the other metalloproteinases.

Agents designed or selected to interact with MMP-13 must be capable of both physically and structurally associating with MMP-13 *via* various covalent and/or non-covalent molecular interactions, and of assuming a three

dimensional configuration and orientation that complements the relevant active site of the MMP-13 molecule.

Accordingly, using these criteria, the structural coordinates of the MMP-13:Compound A complex as disclosed herein, and/or structural coordinates derived therefrom using molecular replacement analysis or homology modeling, agents may be designed to increase either or both of the potency and selectivity of known inhibitors or activators, either by modifying the structure of known inhibitors or activators or by designing new agents *de novo* via computational inspection of the three dimensional configuration and electrostatic potential of an MMP-13 active site.

Accordingly, in one embodiment of the invention, the structural coordinates of Figures 4 or 5 of the present invention, or structural coordinates derived therefrom using molecular replacement or homology modeling techniques as discussed above, are used to screen a database for agents that may act as potential inhibitors or activators of MMP-13 activity (or the activity of MMP-13 analogues). Specifically, the obtained structural coordinates of the present invention are read into a software package and the three dimensional structure is analyzed graphically. A number of computational software packages may be used for the analysis of structural coordinates, including, but not limited to, Sybyl (Tripos Associates), QUANTA and XPLOR (Brunger, A.T., (1993) XPLOR Version 3.1 Manual, Yale University, New Haven, CT). Additional software programs check for the correctness of the coordinates with regard to features such as bond and atom types. If necessary, the three dimensional structure is modified and then energy minimized using the appropriate software until all of the structural parameters are at their equilibrium/optimal values. The energy minimized structure is superimposed against the original structure to make sure there are no significant deviations between the original and the energy minimized coordinates.

The energy minimized coordinates of MMP-13 complexed with a "solved" inhibitor or activator are then analyzed and the interactions between the solved ligand and MMP-13 are identified. The final MMP-13 structure is

modified by graphically removing the solved inhibitor or activator so that only MMP-13 and a few residues of the solved agent are left for analysis of the binding site cavity. QSAR and SAR analysis and/or conformational analysis may be carried out to determine how other inhibitors or activators compare to the solved inhibitor or activator. The solved agent may be docked into the uncomplexed structure's binding site to be used as a template for data base searching, using software to create excluded volume and distance restrained queries for the searches. Structures qualifying as hits are then screened for activity using standard assays and other methods known in the art.

Further, once the specific interaction is determined between the solved inhibitor or activator, docking studies with different inhibitors or activators allow for the generation of initial models of new inhibitors or activators in complex with MMP-13. The integrity of these new models may be evaluated a number of ways, including constrained conformational analysis using molecular dynamics methods (*i.e.*, where both MMP-13 and the complexed activator or inhibitor are allowed to sample different three dimensional conformational states until the most favorable state is reached or found to exist between the protein and the complexed agent). The final structure as proposed by the molecular dynamics analysis is analyzed visually to make sure that the model is in accord with known experimental SAR based on measured binding affinities. Once models are obtained of the original solved agent bound to MMP-13 and computer models of other molecules bound to MMP-13, strategies are determined for designing modifications into the activators or inhibitors to improve their activity and/or enhance their selectivity.

Once an MMP-13 binding agent has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its selectivity and binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the

original group. Such substituted chemical compounds may then be analyzed for efficiency of fit to MMP-13 by the same computer methods described in detail above.

Alternatively, the present invention provides a method for identifying a potential inhibitor or activator that is selective for one or more members of the matrix metalloproteinase family except MMP-13, comprising the steps of (i) using the three dimensional structures of MMP-13 and the desired target matrix metalloproteinase(s) as defined by the relative structural coordinates of amino acids encoding MMP-13 and the target matrix metalloproteinase(s) in order to design or select such a potential inhibitor or activator, and (ii) synthesizing or obtaining said potential inhibitor or activator. In this case, the potential inhibitor or activator is designed to incorporate chemical or steric features favorable for association with an active site of the desired matrix metalloproteinase(s) and unfavorable for association with an MMP-13 active site, preferably where said active site comprises the MMP-13 S1' pocket. The inhibitor or activator may be selected by screening an appropriate database, may designed *de novo* by analyzing the steric configurations and charge potentials of empty MMP-13/matrix metalloproteinase active sites in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors or activators to MMP-13 or other collagenases in order to create "hybrid" activators or inhibitors.

Various molecular analysis and rational drug design techniques are further disclosed in U.S. Patent Nos. 5,834,228, 5,939,528 and 5,865,116, as well as in PCT Application No. PCT/US98/16879, published as WO 99/09148, the contents of which are hereby incorporated by reference.

The present invention may be better understood by reference to the following non-limiting Examples. The following Examples are presented in order to more fully illustrate the preferred embodiments of the invention, and should in no way be construed as limiting the scope of the present invention.

Example 1

^{1}H, ^{15}N and ^{13}CO Assignments and Secondary Structure Determination of MMP-13 Complexed with Compound A

Methods and Results: The uniform ^{15}N and ^{13}C- labeled 165 amino-acid catalytic fragment of human collagenase-3 (MMP-13) was expressed in *E. coli* strain BL21(DE3) containing the plasmid pProMMP-13 according to a published method (Freije *et al.*, J. Biol. Chem. 1994). MMP-13 was purified as previously described (Moy *et al.*, J. Biomol. 1997) with minor modifications. N-terminal amino acid sequencing was performed to confirm the protein's identity while the uniform ^{15}N and ^{13}C labeling of MMP-13 was confirmed by MALDI-TOF mass spectrometry (PerSeptive Biosystems). The sulfonamide derivative of the hydroxamic acid compound, N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-methyl-benzamide, was prepared from 2-amino-3-methyl-benzoic acid methyl ester and p-methoxybenzenesulfonyl chloride followed by alkylation with 3-picolyl chloride, hydrolysis (LiOH/THF) to afford the carboxylic acid and conversion to the hydroxamic acid (oxalyl chloride/DMF/NH2OH). Formation of the HCl salt yielded Compound A as shown in Figure 3.

The NMR samples contained 1 mM of MMP-13 determined spectrophotometrically in a equimolar complex with Compound A in a buffer containing 10 mM deuterated Tris-Base, 100 mM NaCl, 5 mM $CaCl_2$, 0.1 mM $ZnCl_2$, 2 mM NaN_3, 10 mM deuterated DTT, in either 90% H_2O/ 10% D_2O or 100% D_2O at pH 6.5. All NMR spectra were recorded at 35°C on a Bruker AMX-2 600 spectrometer equipped with a triple-resonance gradient probe.

Spectra were processed using the NMRPipe software package (Delaglio *et al.*, J. Biomol. NMR 1995) and analyzed with PIPP (Garrett *et al.*, J. Magn. Reson. 1991), NMRPipe and PEAK-SORT, an in-house software package. The assignments of the ^{1}H, ^{15}N, ^{13}CO, and ^{13}C resonances were based on the following experiments: CBCA(CO)NH, CBCANH, C(CO)NH, HC(CO)NH,

HBHA(CO)NH, HNCO, HCACO, HNHA, HNCA, HCCH-COSY and HCCH-TOCSY (for reviews, see Bax *et al.*, Methods Enzymol. 1994; and Clore & Gronenborn, Methods Enzymol. 1994). The accuracy of the MMP-13 NMR assignments was further confirmed by sequential NOEs in the ^{15}N-edited NOESY-HSQC spectra.

Prior to analysis of the MMP-13 NMR structure, the structure determination of the inhibitor-free catalytic fragment of MMP-1 has been reported (Moy *et al.*, Biochemistry 1998; Moy *et al.*, J. Biomol. NMR 1997)(30 simulated annealing structures deposited with Protein Data Bank, Accession No. 1AYK; restrained minimized mean structure deposited with Protein Data Bank, Accession No. 2AYK). Because the MMPs are highly autocatalytic, the NMR analysis of the inhibitor-free MMP-1 was accomplished by establishing buffer conditions where the enzyme was still active but the rate of self-cleavage of the enzyme had been diminished. This was achieved by the addition of DTT which significantly diminished self-aggregation of the enzyme and by lowering the pH of the sample to 6.5, just above the pH where the enzyme was known to be inactivated because of the loss of the catalytic zinc. Under these conditions, an MMP-1 NMR sample was typically stable for 1-2 months. Unfortunately this was not the case for MMP-13, the protein rapidly degraded within a few hours which required the use of an inhibitor to assign the MMP-13 NMR resonances.

The secondary structure of the MMP-13:Compound A complex is based on characteristic NOE data involving the NH, Hα and Hβ protons from ^{15}N-edited NOESY-HSQC and ^{13}C-edited NOESY-HMQC spectra, ^{3}JHNα coupling constants from HNHA, slowly exchanging NH protons and ^{13}Cα and ^{13}Cβ secondary chemical shifts (for reviews, see Wishart & Sykes, Methods Enzymol. 1994; and Wuthrich, NMR of Proteins and Nucleic Acids, John Wiley & Sons, New York 1986). It was determined that the MMP-13 NMR structure in the complex is composed of three α-helices corresponding to residues 28-44 (a_α), 112-123 (a_β) and 153-163 (a_C) and a mixed parallel and anti-parallel β-sheet consisting of 5 strands corresponding to residues 83-86 (β_1), 95-100 (β_2), 59-66 (β_3), 14-20 (β_4) and 49-53 (β_5). This is essentially identical to the secondary structure observed for other MMP structures.

There were three distinct regions in the MMP-13:Compound A spectra where the resonance assignments are incomplete. These correspond to residues G70-Y73, P87-N91 and T144-H148. Residues T144-H148 correspond to part of the dynamic loop region previously seen in the MMP-1 structure (Moy *et al.*, J. Biomol. NMR 1997). This suggests a similar dynamic profile for this region in the MMP-13 structure even in the presence of a high-affinity inhibitor (IC_{50} = 33 nM). Residues P87 to N91 contain a cluster of prolines which disrupt the sequential assignment process because of the missing NH. Residues G70 to Y73 correspond to a loop region in the vicinity of the structural zinc which was readily assigned in the MMP-1 structure. The backbone and side-chain ^{1}H, ^{15}N, ^{13}C, and ^{13}CO assignments are essentially complete for the remainder of the protein.

Example 2

High Resolution Solution Structure of the Catalytic Fragment of MMP-13 Complexed with Compound A

Materials and Methods:

Preparation of Compound A: The sulfonamide derivative of the hydroxamic acid compound, Compound A, was prepared according to the procedure noted in Example 1 to yield the compound of Figure 3.

Expression of recombinant ^{15}N and $^{13}C/^{15}N$-labeled MMP-13: A 169-residue C-terminally truncated human collagenase-3 (MMP-13) was expressed in *E. coli*. The coding sequence of a C-terminally truncated procollagenase was amplified by PCR from the plasmid pNot3a, that contains the entire coding sequence of MMP-13 (Frieje, *et al.*, J. Biol. Chem. 1994). The PCR primers contained the appropriate restriction sites for ease of cloning. The construct codes for a truncated proMMP-13 with an N-terminal methionine added and a C-terminal proline at residue 169 of the native proMMP-13 sequence. The PCR amplified DNA fragment was the cloned into pET-21a (+) at the Nde I/Sal I sites ,

resulting in a recombinant plasmid designated as pProMMP-13. *E. coli* bacteria, BL21(DE3), containing the plasmid pProMMP-13, were grown in LB broth supplemented with 100 μg/ml ampicilin. An overnight culture was diluted 1:20 and grown at 37°C to an A_{600} of 0.6-0.8 with vigorous shaking. Isopropyl β-D-galactoside (IPTG) was added to a final concentration of 1 mM and cultures were shaken for 3 h at 37°C. The cells were harvested by centrifugation (7000 Xg for 15 min) at 4°C, washed with PBS, and frozen at -70°C until further use.

Uniform ^{15}N and ^{13}C- labeled ProMMP-13 was obtained by growing BL21(DE3) E. coli in defined media containing 2.0 g/l [$^{13}C6$, 98%+]D-glucose and 1.0 g/l [^{15}N, 98%+] ammonium chloride as the sole carbon and nitrogen sources, respectively. In addition, the defined media contained M9 salts (Sambrook, *et al.*, Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Laboratory Press, New York, NY 1989), trace elements, vitamins and 100 μg/ml ampicilin. Conditions for induction and growth were the same as above.

Purification of recombinant ^{15}N and ^{13}C MMP-13: MMP-13 was purified according to Moy *et al.*, J. Biomol. NMR 1997, with modifications as follows. Frozen cell pellets were thawed on ice. Cells were resuspended by homogenization in lysis buffer (0.1 M Tricine, pH 8.0, 10 mM EDTA, 2mM DTT, 0.5 mM PMSF). Cells were lysed by French Press (2X) followed by treatment with lysozyme (1 mg/ml; final) at room temperature for 30 min. The lysate was centrifuged at 45,000 x g for 30 minutes. The pellet was washed twice with 50 mM Tricine pH 7.5, 0.2 M $NaCl_2$, 0.5% Triton X-100, resuspended in fresh urea buffer (20 mM Tricine, pH 7.5, 8 M urea, 0.2% NaN_3, 2 mM DTT) and incubated at room temperature for 1 hour. The urea solubilized protein was centrifuged at 45,000 x g for 30 min and the resultant supernatant was filtered and applied to a Hitrap-Q Sepharose (Pharmacia Biotech) anion exchange column equilibrated in 6 M urea buffer. The column was washed with urea buffer and eluted with a 0-0.25 M NaCl linear gradient. Fractions containing proMMP-13 were detected by SDS-PAGE, pooled and quickly diluted into 5-fold excess of renaturing buffer

(50 mM Tricine, pH 7.5, 0.4 M NaCl, 10 mM $CaCl_2$, 0.1 mM $ZnOAc_2$, 0.02% NaN_3). After 2 days of dialysis against 25 volumes of renaturing buffer (with three changes), refolded proMMP-13 was concentrated to about 4-10 mg/ml in a Millipore Biomax 5 concentrator. ProMMP-13 was activated to MMP-13CAT (catalytic domain) by an overnight incubation at 37 °C in the presence of 1 mM *p*-aminophenylmercuric acetate (APMA).

The activated protein is then applied onto a Superdex-75 16/60 gel filtration column equilibrated in 2.5 mM Tris-HCl, pH 7.5, 5 mM $CaCl_2$, 0.4 M NaCl, 2 mM DTT, 0.02% NaN_3 and 0.05 mM $ZnOAc_2$. The protein is eluted and fractions containing MMP-13CAT were identified by SDS-PAGE. Peak fractions were pooled and the protein was concentrated in a Millipore Biomax concentrator to about 5 mg/ml and stored at -70 °C. N-terminal amino acid sequencing was performed to confirm the protein's identity. The uniform ^{15}N and ^{13}C labeling of MMP-13-CAT was confirmed by MALDI-TOF mass spectrometry (PerSeptive Biosystems).

NMR Sample Preparation: The MMP-13:Compound A NMR sample contained 1mM ^{15}N-or $^{15}N/^{13}C$-labeled MMP-13 with Compound A in a 1:1 ratio. The sample was prepared by repeated buffer exchange using 20-30ml solution containing 10mM deuterated Tris-Base, 100mM NaCl, 5mM $CaCl_2$, 0.1mM $ZnCl_2$, 2mM NaN_3, 10mM deuterated DTT, and 0.2mM Compound A in either 90% H_2O/10 % D_2O or 100% D_2O. Buffer exchange was carried out on a Millipore Ultrafree-15 Centrifugal Filter Unit. Excess Compound A was removed by additional buffer exchanges where Compound A was removed from the buffer.

NMR Data Collection: All spectra were recorded at 35°C on a Bruker AMX-2 600 spectrometer using a gradient enhanced triple-resonance $^1H/^{13}C/^{15}N$ probe. For spectra recorded in H_2O, water suppression was achieved with the WATERGATE sequence and water-flip back pulses (Piotto, *et al.*, J. Biomol. NMR 1992; Grzesiek and Bax, J. Am. Chem. Soc. 1993). Quadrature detection in the

indirectly detected dimensions were recorded with States-TPPI hypercomplex phase increment (Marion, *et al.*, J. Magn. Reson. 1989). Spectra were collected with appropriate refocusing delays to allow for 0,0 or -90,180 phase correction.

The resonance assignments and bound conformation of Compound A in the MMP-1: Compound A complex were based on the 2D $^{12}C/^{12}C$-filtered NOESY (Petros, *et al.*, FEBS Lett. 1992; Gemmecker, *et al.*, J. Magn. Reson. 1992), 2D $^{12}C/^{12}C$-filtered TOCSY (Petros, *et al.*, FEBS Lett. 1992; Gemmecker, *et al.*, J. Magn. Reson. 1992) and $^{12}C/^{12}C$-filtered COSY experiments (Ikura and Bax, J. Magn. Reson. 1992).

The MMP-13:Compound A structure is based on the following series of spectra: HNHA (Vuister and Bax, J. Am. Chem. Soc. 1993), HNHB (Archer, *et al.*, J. Magn. Reson. 1992), 3D long-range ^{13}C-^{13}C correlation (Bax and Popchapsky, J. Magn. Reson. 1992), coupled CT-HCACO (Powers, *et al.*, J. Magn. Reson. 1991; Vuister, *et al.*, J. Am. Chem. Soc. 1992), HACAHB-COSY (Grzesiek, *et al.*, J. Amer. Chem. Soc. 1995), 3D ^{15}N- (Mario, *et al.*, Biochemistry 1989; Zuiderweg and Fesik, Biochemistry 1989) and ^{13}C-edited NOESY (Zuiderweg, *et al.*, J. Magn. Reson. 1990; Ikura, *et al.*, J. Magn. Reson. 1990), and 3D ^{13}C-edited/^{12}C-filtered NOESY (Lee, *et al.*, FEBS Lett. 1994). experiments. The ^{15}N-edited NOESY, ^{13}C-edited NOESY and 3D ^{13}C-edited/^{12}C-filtered NOESY experiments were collected with 100 msec, 120 msec and 110 msec mixing times, respectively. The acquisition parameters for each of the experiments used in determining the solution structure of MMP-13 complexed with Compound A were as reported previously (Moy, *et al.*, Biochemistry, 1998).

Spectra were processed using the NMRPipe software package (Delaglio, *et al.*, J. Biomol. NMR, 1995) and analyzed with PIPP (Garrett, *et al.*, J. Magn. Reson., 1991) on a Sun Sparc Workstation. When appropriate, data processing included a solvent filter, zero-padding data to a power of two, linear predicting back one data point of indirectly acquired data to obtain zero phase corrections, linear prediction of additional points for the indirectly acquired dimensions to increase resolution. Linear prediction by the means of the mirror

image technique was used only for constant-time experiments (Zhu and Bax, J. Magn. Reson., 1992). In all cases data was processed with a skewed sine-bell apodization function and one zero-filling was used in all dimensions.

Interproton Distance Restraints: The NOEs assigned from 3D ^{13}C-edited/^{12}C-filtered NOESY and 3D ^{15}N-edited NOESY experiments were classified into strong, medium, and weak corresponding to interproton distance restraints of 1.8-2.7 Å (1.8-2.9 Å for NOEs involving NH protons), 1.8-3.3 Å (1.8-3.5 Å for NOEs involving NH protons), and 1.8-5.0 Å , respectively (Williamson, *et al.*, J. Mol. Biol., 1985; Clore, *et al.*, EMBO J., 1986). Upper distance limits for distances involving methyl protons and non-stereospecifically assigned methylene protons were corrected appropriately for center averaging (Wuthrich, *et al.*, J. Mol. Biol., 1983).

Torsion Angle Restraints and Stereospecific Assignments. The β-methylene stereospecific assignments and χ_1 torsion angle restraints were obtained primarily from a qualitative estimate of the magnitude of $^3J_{\alpha\beta}$ coupling constants from the HACAHB-COSY experiment (Grzesiek, *et al.*, J. Am. Chem. Soc., 1992) and $^3J_{N\beta}$ coupling constants from the HNHB experiment (Archer, *et al.*, J. Magn. Reson., 1991). Further support for the assignments was obtained from approximate distance restraints for intraresidue NOEs involving NH, CαH, and CβH protons (Powers, *et al.*, Biochemistry, 1993).

The ϕ and ψ torsion angle restraints were obtained from $^3J_{NH\alpha}$ coupling constants measured from the relative intensity of Hα crosspeaks to the NH diagonal in the HNHA experiment (Vuister and Bax, J. Am. Chem. Soc. 1993), from a qualitative estimate of the magnitude of $^3J_{\alpha\beta}$ coupling constants from the HACAHB-COSY experiment (Grzesiek, *et al.*, J. Am. Chem. Soc., 1992) and from approximate distance restraints for intraresidue and sequential NOEs involving NH, CαH, and CβH protons by means of the conformational grid search program STEREOSEARCH (Nilges, *et al.*, Biopolymers 1990), as described previously (Kraulis, *et al.*, Biochemistry 1989). $^1J_{c\alpha H\alpha}$ coupling

constants obtained from a coupled 3D CT-HCACO spectrum were used to ascertain the presence of non-glycine residues with positive f backbone torsion angles (Vuister, *et al.*, J. Am. Chem. Soc. 1992). The presence of a $^{1}J_{c\alpha H\alpha}$ coupling constant greater then 130 Hz allowed for a minimum ϕ restraint of -2° to -178°.

The Ile and Leu $\chi 2$ torsion angle restraints and the stereospecific assignments for leucine methyl groups were determined from $^{3}J_{C\alpha C\delta}$ coupling constants obtained from the relative intensity of Cα and Cδ cross peaks in a 3D long-range ^{13}C-^{13}C NMR correlation spectrum (Bax, *et al.*, J. Am. Chem. Soc. 1992), in conjunction with the relative intensities of intraresidue NOEs (Powers, *et al.*, Biochemistry 1993). Stereospecific assignments for valine methyl groups were determined based on the relative intensity of intraresidue NH-CγH and CαH-CγH NOEs as described by Zuiderweg *et al.* (1985) (Zuiderweg, *et al.*, Biopolymers 1985). The minimum ranges employed for the ϕ, ψ, and χ torsion angle restraints were ± 30°, ± 50°, and ± 20°, respectively (Kraulis, *et al.*, Biochemistry 1989).

Structure Calculations: The structures were calculated using the hybrid distance geometry-dynamical simulated annealing method of Nilges *et al.* (1988) (Protein Eng.) with minor modifications (Clore, *et al.*, Biochemistry 1990) using the program XPLOR (Brunger, X-Plor Version 3.1 Manual, Yale University, New Haven, CT), adapted to incorporate pseudopotentials for $^{3}J_{NH\alpha}$ coupling constants (Garrett, *et al.*, J. Magn. Reson. Ser. B 1994), secondary $^{13}C\alpha/^{13}C\beta$ chemical shift restraints (Kuszewski, *et al.*, J. Magn. Reson. Ser B 1995) and a conformational database potential (Kuszewski, *et al.*, Protein Sci. 1996; Kuszewski, *et al.*, J. Magn. Reson. 1997). The target function that is minimized during restrained minimization and simulated annealing comprises only quadratic harmonic terms for covalent geometry, $^{3}J_{NH\alpha}$ coupling constants and secondary $^{13}C\alpha/^{13}C\beta$ chemical shift restraints, square-well quadratic potentials for the experimental distance and torsion angle restraints, and a quartic van der Waals term for non-bonded contacts. All peptide bonds were constrained to be

planar and trans. There were no hydrogen-bonding, electrostatic, or 6-12 Lennard-Jones empirical potential energy terms in the target function.

To prevent the Zn and Ca ions from being expelled during the high-temperature simulated annealing stages of the refinement protocol, a minimal number of distance restraints between the His sidechain and Zn and between backbone atoms and Cα were included in the XPLOR distance restraint file based on the observed coordination in the X-ray structures (Lovejoy, *et al.*, Science 1994; Lovejoy, *et al.*, Biochemistry 1994; Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994; Borkakoti, *et al.*, Nat. Struct. Biol. 1994).

The starting MMP-13:Compound A complex structure for the simulated-annealing protocol was obtained by manually docking Compound A into a homology model for MMP-13. The initial orientation of Compound A in the MMP-13 active site was based on the previously reported MMP-1:CGS-27023A structure (Moy, *et al.*, Biochemistry 1999).

Homology modeling methods were utilized to generate a three dimensional model of MMP-13. The linear amino acid sequence corresponding to the catalytic domain of MMP-13 was aligned (SYBYL) with the catalytic domains of MMP-1, MMP-7 and MMP-8 based on the availability of their x-ray crystallographic structures (Bode, *et al.*, EMBO J 1994; Spurlino., Proteins: Struct., Funct., Genet. 1994; Betz, *et al.*, Eur. J. Biochem. 1997; Lovejoy, *et al.*, Nat. Struct. Biol. 1999; Borkakoti, *et al.*, Nat. Struct. Biol. 1994; Browner, *et al.*, Biochemistry 1995). The alignments of MMP-13 with MMP-1 and MMP-8 demonstrated the highest homology where the computed identities are 58.9% and 61.4%, respectively (Figure 2).

The X-ray structure of MMP-8 was selected to be used as the template for homology modeling the structure of MMP-13. This decision was based mainly on the sequence alignment shown in Figure 2B where no insertions (labeled "###") are found in the critical specificity loop (Labeled Underlined and Boldface). In Figure 2A, the region labeled "##" in the specificity loop shows that there is an "insertion" of 2 additional amino acid residues compared to the sequence length of MMP-1. Based on our analysis of

the alignments, MMP-8 would allow for a more accurate modeling of the inhibitor binding pockets since no predictions have to be made within this loop region.

COMPOSER (SYBYL) was used to construct the initial homology model of MMP-13. The only insertion was a serine (labeled '**' in Figure 2B) at position 32 of MMP-13. The insertion of S32 occurs within a coiled region which is at the entrance of a long alpha helix and about 17 angstroms from the S' specificity loop. The model of MMP-13 was then energy minimized utilizing a set of nested refinement procedures (Chen, *et al.*, J. Biomol. Struct. Dyn. 1995), but where the protein backbone heavy atoms were constrained as close as possible to their original positions.

The MMP-13:Compound A model was then subjected to a 1000 steps of CHARMM minimization with the 5 intramolecular NOE restraints and the 47 distance restraints observed between MMP-13 and Compound A where the coordinates for MMP-13 were kept fixed. This approach approximated the positioning of Compound A in the active site of MMP-13 without distorting the MMP-13 structure. The final structure was exported as a PDB file and used as the starting point for XPLOR simulated annealing protocol where all the residues in the structure were free to move. Since the initial stage of the simulated annealing protocol corresponds to high-temperature dynamics (1500 K) with a relatively weak XPLOR NOE force constant (Ries and Petrides, Biol. Chem. Hoppe-Seyler 1995), the initial MMP-13:Compound A structure does not bias the structure determination process since the structure is effectively free to explore the available conformational space. Additionally, each iteration of the simulated annealing process begins with a random trajectory for the molecular dynamics. The fact that these trajectories differ by upwards of 10 Å assures a distinct exploration of conformational space for the ensemble of MMP-13:Compound A structures determined from the simulated annealing protocol.

Results and Discussion

Compound A Resonance Assignments and Bound Conformation: The primary structure of Compound A along with the proton naming convention is shown in Figure 3. The NMR assignments for Compound A in the MMP-13 complex followed established protocols using 2D ^{12}C-filtering experiments (Petros, *et al.*, FEBS Lett. 1992; Gemmecker, *et al.*, J. Magn. Reson. 1992; Ikura and Bax, J. Am. Chem. Soc. 1992) since the NMR sample was composed of $^{13}C/^{15}N$ labeled MMP-13 and unlabeled Compound A. Thus, traditional 2D-NOESY, COSY and TOCSY spectra of Compound A in the presence of MMP-13 yielded straightforward assignments for Compound A along with assignments for free Compound A (data not shown). The only notable difference in the assignments for free and bound Compound A is the observation of two distinct resonances for 2HB1/2 in the complex (4.91 ppm; 4.67 ppm). The missing resonance in the free Compound A may simply be obscured by water. Also, an observation that the protons on the p-methoxyphenyl ring are degenerate suggests rapid ring flips when complexed to MMP-13. This was also seen with CGS-27023A complexed with both MMP-1 and stromelysin (Gonnella, *et al.*, Bioorg. Med. Chem. 1997; Moy, *et al.*, Biochemistry 1998; Moy, *et al.*, Biochemistry 1999).

Compound A does not adopt a preferred conformation in the absence of MMP-13 as evident by the lack of structural NOEs. Only a minimal number of intramolecular NOEs were observed for Compound A in the MMP-13 complex which were relevant to the bound conformation of Compound A (data not shown). The minimal number of structural NOEs is a result of the Compound A conformation, structure and chemical shift degeneracy. A number of the observed NOEs correspond to a sequential interaction which have no effect on the overall conformation of the inhibitor and were not used in the refinement of Compound A or the complex. The structural intramolecular NOEs observed are primarily between 1HH* and the pyridine ring and between 2HB1/2 and both the p-methoxyphenyl and aryl ring. These NOEs are consistent with the "splayed" conformation previously observed for CGS-27023A bound to both MMP-1 and stromelysin, but the bound conformation of

Compound A is predominately determined from the intermolecular NOEs between Compound A and MMP-13 (Table 1).

Structure Determination: The NMR structure determination methodology is an iterative procedure where the current state of the structure is used to analyze the ambiguous NOE data. In essence, the structure is used as a distance filter to sort through the ambiguous NOE list where the first structure is determined from unambiguous data. For the refinement of MMP-13, the initial structure was a homology model based on the MMP-8 X-ray structure. This was justified by the overall similarity in previously reported MMP structures and from the secondary structure assignments by NMR for MMP-13. The regular secondary structure elements of MMP-13 were identified from a qualitative analysis of sequential and inter-strand NOEs, NH exchange rates, ^{3}JHNα coupling constants (Clore, *et al.*, Crit. Rev. Biochem. Mol. Biol. 1989) and the $^{13}C\alpha$ and $^{13}C\beta$ secondary chemical shifts (Spera and Bax, J. Am. Chem. Soc. 1991). The deduced secondary structure is essentially identical to the inhibitor-free MMP-1 NMR structures previously reported.

The final 30 simulated annealing structures calculated for residues 7-164 were based on 3279 experimental NMR restraints, consisting of 2561 approximate interproton distance restraints, 51 distance restraints between MMP-13 and Compound A, 88 distance restraints for 44 backbone hydrogen bonds, 391 torsion angle restraints, 103 $^{3}J_{NH\alpha}$ restraints 123 Cα restraints and 108 Cβ restraints. Stereospecific assignments were obtained for 81 of the 100 residues with β-methylene protons, for the methyl groups of 5 of the 6 Val residues, and for the methyl groups of 12 of the 13 Leu residues. In addition, 12 out of the 12 Phe residues and 7 out of the 8 Tyr residues were well defined making it possible to assign NOE restraints to only one of the pair of CδH and CεH protons and to assign a χ2 torsion angle restraint. Similarly, χ2 torsion angle restraints were assigned for the three Trp residues. The atomic rms distribution of the 30 simulated annealing structures about the mean coordinate positions for residues 7-164 is 0.43 ± 0.06 Å for the backbone atoms, 0.81 ±

0.09 Å for all atoms, and 0.47 ± 0.04 Å for all atoms excluding disordered surface side chains. The mean standard deviation for the ϕ and ψ backbone torsion angles of residues 7-164 are 6.2 ± 11.3° and 7.1 ± 11.8°, respectively. The high quality of the MMP-13 NMR structure is also evident by the results of PROCHECK analysis and by a calculated, large negative value for the Lennard-Jones-van der Waals energy (-695 ± 11 kcal mol^{-1}). For the PROCHECK statistics, an overall G-factor of 0.16 ± 0.16, a hydrogen bond energy of 0.82 ± 0.05 and only 7.8 ± 1.0 bad contacts per 100 residues are consistent with a good quality structure comparable to ~1Å X-ray structure.

The high quality of the MMP-13 NMR structure is also evident by the very small deviations from idealized covalent geometry, by the absence of interproton distance and torsion angle violations greater than 0.1 Å and 1°, respectively and by the fact that most of the backbone torsion angles for non-glycine residues lie within expected regions of the Ramachandran plot (not shown). 91.5% of the residues lie within the most favored region of the Ramachandran ϕ, ψ plot and 7.8% in the additionally allowed regions. $^1JC\alpha H\alpha$ coupling constants from the coupled CT-HCACO experiment indicated that all non-glycine residues have negative ϕ torsion angles.

The quality of the NMR data to properly define the complex is also supported by the well-defined coordinates for Compound A and the active site residues, where the atomic rms distribution is 0.47 ± 0.08Å and 0.18 ± 0.03 Å for the heavy atoms of Compound A and MMP-13 backbone atoms, respectively.

Description of the MMP-13:Compound A Structure: The overall fold of MMP-13 is essentially identical to previously reported MMP structures (Bode, *et al.*, EMBO J. 1994; Gooley, *et al.*, Nat. Struct. Biol. 1994; Lovejoy, *et al.*, Science 1994; Lovejoy, *et al.*, Ann. N. Y. Acad. Sci. 1994; Lovejoy, *et al.*, Biochemistry 1994; Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994; Stams, *et al.*, Nat. Struct. Biol. 1994; Becker, *et al.*, Protein Sci. 1995; Gonnella, *et al.*, Proc. Natl. Acad. Sci. U. S. A. 1995; Van Doren, *et al.*, Protein Sci. 1995; Botos, *et al.*, Proc. Natl. Acad. Sci. USA 1996; Broutin, *et al.*, Acta Crystallogr., Sect. D: Biol. Crystallogr.

1996; Gooley, *et al.*, J. Biomol. NMR 1996; Betz, *et al.*, Eur. J. Biochem. 1997; Gonnella, *et al.*, Bioorg. Med. Chem. 1997; Moy, *et al.*, Biochemistry 1998 and Moy, *et al.*, Biochemistry 1999). The MMP-13 NMR structure is composed of three α-helices corresponding to residues 28-44 (α_A), 112-123 (α_B) and 153-163 (α_C) and a mixed parallel and anti-parallel b-sheet consisting of 5 strands corresponding to residues 83-86 (β_1), 95-100 (β_2), 59-66 (β_3), 14-20 (β_4) and 49-53 (β_5). The active site of MMP-13 is bordered by β-strand IV, the Ca^{+2} binding loop, helix B and a random coil region from residues P139-Y141. The catalytic zinc is chelated by H119, H123, and H129 while the structural zinc is chelated by H69, H84 and H97. The calcium ion is chelated in a loop region consisting of residues D75 to G79. An interesting feature of the MMP active-site structure is an apparent kink in the backbone that occurs between the Ca^{+2} binding loop and β-strand IV. In the case of MMP-13, this results in the NHs of both L82 and A83 facing toward the active site of the enzyme. An important feature of substrate and inhibitor binding to the MMPs are hydrogen bonding interactions with β-strand IV which is facilitated by this unusual kink conformation (Lovejoy, *et al.*, Science 1994; Lovejoy, *et al.*, Biochemistry 1994; Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994; and Borkakoti, *et al.*, Nat. Struct. Biol. 1994).

The interaction of Compound A in the active site of MMP-13 was determined by 5 intramolecular NOEs for Compound A and by a total of 47 intermolecular distance restraints between MMP-13 and Compound A. The key MMP-13 residues involved in the interaction with the inhibitor correspond to three distinct MMP-13 regions: residues L81, L82 and A83 from β-strand IV; residues L115, V116, and H119 from α-helix II; and L136, I140 and Y141 from the active site loop which comprise the S1' and S2' pockets of MMP-13. A unique feature of the MMP-13 structure is the large S1' pocket which nearly reaches the surface of the protein.

Compound A binds to the right-side of the catalytic Zn where the p-methoxyphenyl of Compound A sits in the S1' pocket of the MMP-13 active site. This positioning is evident from the observed NOEs from 3HH*, 3HE1/2

and 3HD1/2 to L115, V116, H119, L136, and Y141. The aryl group primarily interacts with the side-chain of L81 as evident by the strong NOEs between 1HH*, 1HE2 and 1HZ and the L81 spin-system. Finally, the pyridine ring is essentially solvent exposed but interacts with the side-chain of I140. These interactions position Compound A such that the hydroxamic acid moiety of Compound A chelates to the "right" of the catalytic zinc and the sulfonyl oxygens are in hydrogen-bonding distance to the backbone NH of L82.

It is interesting to note that the active site loop is highly dynamic in both the inhibitor-free and CGS-27023A structures based on S^2 order-parameters (Moy, *et al.*, J. Biomol. NMR 1997). This region in the MMP-13:Compound A structure appears to be significantly less mobile by the observation that most of the residues in this loop region were easily observable in the ^1H-^{15}N HSQC spectra and readily assigned. One possible explanation for this difference is the hydrophobic interaction between the pyridine ring of Compound A and the side-chain for Ile-140. In MMP-1, I140 is replaced by a serine which essentially eliminates this beneficial interaction.

Another unique feature of the MMP-13 NMR structure is the apparent dynamic nature of residues H69 to Y73. These residues are completely disordered due to the lack of any assignment information and the resulting absence of any constraint information presumably a result of the flexible nature of these residues. Residues H69 to Y73 occur between the Ca^{+2} binding loop and the structural zinc where the corresponding region in the previously solved MMP-1 NMR structures is well defined. There is no apparent explanation for this change in mobility between the two NMR structures but it may contribute to the observed difference in the physical behavior of MMP-1 and MMP-13. Under identical conditions, inhibitor-free MMP-1 is stable for upwards of two months whereas inhibitor-free MMP-13 degrades immediately.

Comparison of the MMP-13:Compound A and MMP-1:CGS-27023A Structures:

The high-resolution NMR structure for the MMP-13:Compound A complex was effectively and efficiently determined by using a homology model based on the

MMP-1 NMR structure as an initial structure to analyze ambiguous NOESY data. This result is evident of the high structural and sequence similarity between members of the MMP family and consistent with the previously observed best-fit superposition of the backbone atoms for MMP-1, stromelysin, matrilysin and neutrophil collagenase (Moy, *et al.*, Biochemistry 1998; Moy, *et al.*, Biochemistry 1999).

The strong similarity between the various MMP structures creates an initial difficulty in designing specific MMP inhibitors. This is exemplified by the high sequence similarity among the MMPs in the active site. Comparison of the sequence similarity between MMP-13 and MMP-1 illustrates this difficulty. There are only a few significant residue differences between the two enzymes where these modifications results in a significant change in the local environment of the active site. The R114 to V115 modification results in a conversion from a hydrophilic to a hydrophobic environment at the base of the S1' pocket between MMP-1 and MMP-13, respectively. Similarly, the N80 to L81 substitution places a bulkier hydrophobic residue in the S2' pocket for MMP-13 compared to a more hydrophilic environment for MMP-1. Similarly in the active loop region, I140 a bulky hydrophobic residue in MMP-13 replaces the smaller hydrophilic S139 residue in MMP-1. Clearly, it is feasible to incorporate substituents into a small molecule to take advantage of these spatial distinct environmental changes between MMP-1 and MMP-13. Nevertheless, when these sequence and environmental differences are averaged across the MMP family it becomes less discriminating and extremely difficult to design an inhibitor to a specific MMP subtype based strictly on the small sequence differences.

Conversely, the most distinct structural difference between the MMPs and readily amenable to incorporating specificity in drug design is the relative size and shape of the S1' pocket. This is clearly evident by comparison of the defined S1' pockets for MMP-13 and MMP-1. The large difference in size in the S1' pockets between the MMP-13 and MMP-1 NMR structures is striking. The S1' pocket for MMP-13 nearly reaches the outer surface of the protein and

is greater then twice the size of MMP-1. The additional size of the MMP-13 S1' pocket relative to MMP-1 is best illustrated by the filling capacity of the two inhibitors. In the MMP-1:CGS-27023A NMR structure, the p-methoxyphenyl effectively fills the available S1' pocket for MMP-1. Conversely, in the MMP-13:Compound A complex the p-methoxyphenyl only partially fills the available space within the MMP-13 S1' pocket. The size of the MMP-13 pocket is actually similar in size to stromelysin where the design of stromelysin inhibitors has taken advantage of this deeper S1' pocket by using a biphenyl substituent in another series instead of the p-methoxyphenyl in Compound A to bind into the S1' pocket (Hajduk, *et al.*, J. Am. Chem. Soc. 1997; Olejniczak, *et al.*, J. Am. Chem. Soc. 1997). Thus, the NMR structures for MMP-13 and MMP-1 suggest that a ready approach to designing specificity between these MMPs is to take advantage of the significantly different sized S1' pockets. The high mobility of the MMP-1 active site presents a potential caveat to this analysis of the static images of the MMP-1 and MMP-13 structures. It is probable that the MMP-1 active site is capable of accommodating a S1' substituent larger then implied from its current structure due to its increased mobility in both free and inhibited structures.

Examination of the binding mode of Compound A in the MMP-13:Compound A complex suggests a conformation generally similar to CGS-27023A in the MMP-1:CGS-27023A NMR structure previously reported (30 simulated annealing structures deposited with Protein Data Bank, Accession No. 4AYK; restrained minimized mean structure deposited with Protein Data Bank, Accession No. 3AYK). Compound A and CGS-27023A are structurally very similar with the only difference being the nature of the substituent binding in the S2' pocket where an aryl group in Compound A replaces the isopropyl group in CGS-27023A. The strong resemblance between the binding mode of Compound A and CGS-27023A is apparent from the nearly identical intermolecular NOE patterns observed between the inhibitors and the proteins. The key MMP-13 residues involved in the interaction with Compound A correspond to L81, L82 and A83 from β-strand IV; residues L115, V116, and

H119 from α-helix II; and L136, I140 and Y141 from the active site loop. Similarly, the MMP-1 residues involved in the interaction with CGS-27023A correspond to residues N80, L81, A82 and H83 from β-strand IV; residues R114, V115, H118 and E119 from α-helix II; and L135, P138, Y137, S139 and Y140 from the dynamic flexible loop.

As stated previously, there are three distinct residue changes between MMP-13 and MMP-1 in the active site. The R114 to L115 change between MMP-1 and MMP-13, respectively, has a significant impact on the environment at the base of the S1' pocket but since Compound A only partially fills the MMP-13 S1' pocket this change should not effect the binding conformation of Compound A relative to CGS-27023A. Conversely, the N80 to L81 substitution directly interacts with the inhibitors in the S2' pocket and may result in an effective change in the binding mode of the inhibitors. To complicate the analysis, the only change in the inhibitors are the substituents that bind the S2' pocket. For the MMP-1:CGS-27023A complex, the isopropyl group interacts with both the sidechains of N80 and H83 where the aryl group from Compound A only interacts with L81 in MMP-13. Additionally, CGS-27023A is in hydrogen-bonding distance to both L81 and A82, whereas Compound A appears to form a bifurcated hydrogen bond with L82. This analysis suggests that CGS-27023A binds closer to β-strand IV since the S2' pocket is more accessible in MMP-1 due to the absence of the bulky L81 side-chain and the presence of the aryl group in Compound A. A direct comparison of the bound conformations suggest only a subtle difference in the relative orientation of the inhibitors. The S139 to I140 difference between MMP-1 and MMP-13, respectively, appears to be related to a mobility change as opposed to a structural change. In the MMP-1:CGS-27023A structure the pyridine ring position is essentially undefined and solvent exposed this compares to the MMP-13:Compound A structure where the pyridine ring binds with the side-chain of I140. Clearly, Ile is a bulkier more hydrophobic group relative to Ser which would provide a beneficial hydrophobic interactions with the pyridine ring. The more interesting observation is the apparent decrease in mobility for the active

loop in the MMP-13 structure which may be related the pyridine ring I140 interaction. This appears to be consistent with previously inhibited MMP X-ray structures (Spurlino, *et al.*, Proteins: Struct., Funct., Genet. 1994) where the inhibitor may extend the formation of a β-sheet between b-strand IV and the active loop region which results in low B-factors in the X-ray structure. This may suggest that the mobility of the active loop region is easily removed with any positive interaction with the inhibitor.

There are apparently some interesting differences between the mode of binding for the two inhibitors in the MMP-13:Compound A and MMP-1:CGS-27023A NMR structures. The more striking observation is the overall similarity between the two structures. Despite some significant sequence differences and a large difference in the size and shape of the S1' pocket either inhibitor structure would accurately predict the other structure. This observation seems to indicate that the major contributing factors to inhibitors binding the MMPs is the fit in the S1' pocket and the binding of the hydroxamic acid to the catalytic zinc. The interaction in the S2' pocket appears to have a more subtle impact on inhibitor binding and selectivity since both Compound A and CGS-27023A are low nanomolar inhibitors of MMP-13 and MMP-1, respectively. Therefore, the high-resolution solution structure of the MMP-13:Compound A in conjunction with the previously reported MMP-1 NMR structures suggest that taking advantage of the significant differences in the size and shape of the S1' pocket is a reasonable approach for developing specific MMP inhibitors.

The studies described herein present the high-resolution solution structure of MMP-13 complexed with a sulfonamide derivative of a hydroxamic acid compound (Compound A). The overall fold of MMP-13 is similar to previously reported MMPs structures. The major difference is the large S1' pocket which nearly reaches the surface of the protein. The structure was based on a total of 3279 constraints including 47 distance restraints between MMP-13 and Compound A from X-filtered NOESY experiments. The inhibitor was found to bind to the "right" side of the catalytic Zn such that the p-methoxyphenyl ring

sits in the S1' pocket, the aryl moiety interacts with L81 of βIV, the pyridine ring interacts with I140 of the active site loop, hydrogen bond interactions exist between the sulfonamide oxygens with residue L82 and the hydroxamic acid chelates the catalytic Zn. This inhibitor binds MMP-13 similarly to the MMP-1: CGS-27023A complex suggesting that appropriately filling the S1' pocket may play a key role in developing selective MMP inhibitors.

Table 1. Observed NOEs Between Compound A and MMP-13

Compound A	MMP-13	NOE Class	Compound A	MMP-1	NOE Class
1HH*	L81 Hγ	W	3HH*	Y141 Hα	M
1HH*	L81 Hδ1#	W	3HH*	Y141 Hβ1	W
1HH*	L81 Hδ2#	M	3HH*	Y141 Hβ2	W
1HH*	L81 Hα	S	3HH*	Y141 Hδ2	W
1HE2	L81 Hδ1#	W	3HE2	L82 Hδ1#	W
1HE2	L81 Hδ2#	M	3HE1	A83 Hβ#	W
1HZ	L81 Hδ1#	W	3HE1	H116 Hα	W
1HZ	L81 Hδ2#	M	3HE1	H116 Hγ1#	M
2HZ	I140 Hγ2#	W	3HE2	H116 Hγ2#	W
2HE1	I140 Hδ1#	W	3HE2	I140 Hγ2#	W
3HH*	L82 Hδ1#	W	3HE2	Y141 Hα	W
3HH*	L115 Hβ#	W	3HE2	Y141 Hβ1	W
3HH*	L115 Hγ	W	3HE2	Y141 Hβ2	W
3HH*	L115 Hδ1#	W	3HD2	L82 Hδ1#	W
3HH*	L115 Hδ2#	W	3HD1	A83 Hβ#	W
3HH*	V116 Hα	W	3HD1	V116 Hγ1#	W
3HH*	V116 Hγ1#	W	3HD2	V116 Hγ2#	W
3HH*	V116 Hγ2#	M	3HD2	I140 Hα	W
3HH*	H119 Hα	W	3HD2	I140 Hγ2#	W
3HH*	H119 Hδ2	W	3HD2	Y141 Hα	W
3HH*	H119 Hβ1	W	3HD2	Y141 Hβ1	W
3HH*	H119 Hβ2	W	3HD2	Y141 Hβ2	W
3HH*	L136 Hδ1#	W	3HD2	Y141 HN	W
3HH*	L136 Hδ2#	W			

Example 3

Structure Based Design of a Novel, Potent, and Selective Inhibitor for MMP-13

The matrix metalloproteinases (MMPs) comprise a family of zinc containing enzymes that cleave a broad range of substrates including collagens, fibronectin and gelatins where the substrate preference various for individual MMPs. The design of MMP inhibitors has been initially based upon imitation of the binding interaction of natural protein substrates to MMPs where structural information of MMPs complexed with peptide substrates has been determined by x-ray crystallography and NMR spectroscopy. This structural information has provided a general description of the MMPs active site.

The active site for the MMPs is composed of a catalytic zinc chelated by three histidines where three substrate binding pockets are located to both the right (S1', S2', S3') and left (S1, S2, S3) of the catalytic zinc. The substrate binding pockets were identified by the interactions of side chains from the peptide substrate with the MMPs. The primary effort in MMP inhibitor design has focused on compounds that chelate the catalytic zinc while primarily binding in the S1' and S2' pockets. This has evolved from the observation that the structural characteristics of the S1' pocket (size, shape, amino acid composition) incurs the greatest variability between the individual MMPs and this provides an obvious approach in designing selective and specific MMP inhibitors. Nevertheless, there has also been success in utilizing the binding pockets to the left of the catalytic zinc in addition to or in combination with the right handed binding pockets in the design of inhibitors.

The underlying challenge in designing MMP inhibitors is the reasonably high sequence and structural homology observed between the individual members of the MMP family making it intrinsically difficult to design an inhibitor that will function against a single MMP in the absence of structural information. The problem with a non-specific MMP inhibitor as a drug is the high likelihood of serious side-effects because of the large number of enzymes in the MMP family and their corresponding diversity in targets and function.

Accordingly, the detailed structural information provided herein is a critical component of an inhibitor design program targeting a particular MMP enzyme.

Materials and Methods:

Synthesis of Compound D and Compound E: The sulfonamide derived from 2-amino-3,5-dimethyl-benzoic acid methyl ester and p-methoxybenzenesulfonyl chloride was N-alkylated with benzyl bromide and the ester group of the resulting intermediate was hydrolyzed (LiOH/THF) to afford the carboxylic acid. The corresponding hydroxamic acid was formed by preparation of the acid chloride (oxalyl chloride/DMF) followed by reaction with hydroxylamine. Compound E was synthesized by reaction of 2-amino-3,5-dimethyl-benzoic acid methyl ester and p-fluorobenzenesulfonyl chloride followed by N-alkylation with benzyl bromide. Hydrolysis of the methyl ester (LiOH/THF) followed by displacement of fluorine with the alkoxide of benzofuran-2-carboxylic acid (2-hydroxy-ethyl)-amide gave, after conversion to the hydroxamic acid and formation of the HCl salt as described above, Compound E.

NMR Sample Preparation: Uniformly (>95%) ^{15}N- and $^{15}N/^{13}C$-labeled human recombinant MMP-13 was expressed in *E. coli* and purified as described previously. 1mM $^{13}C/^{15}N$- and ^{15}N- MMP-13 NMR samples were prepared by concentration and buffer exchange using Millipore Ultrafree -10 centrifugal filters into a buffer containing 10mM deuterated Tris-base, 100mM NaCl, 5mM $CaCl_2$, 0.1 mM $ZnCl_2$, 2 mM NaN_3, 10mM deuterated DTT in 90% H_2O/10% D_20 or 100% D2O. The 10:1 Compound B:MMP-13 samples were prepared by addition of Compound B into either a 1mM $^{13}C/^{15}N$- or ^{15}N-MMP-13 sample followed by pH readjustment. The sample to explore the potential of competitive inhibition between Compound B and Compound A was prepared by first adding 1mM of Compound A to a 1 mM ^{15}N- MMP-13 sample followed by the addition of 10mM Compound B. The initial MMP-13:Compound A sample was made by buffer exchange of ^{15}N- MMP-13 into the buffer containing 0.1 mM Compound A followed by additional buffer exchanges to remove excess

Compound A. Finally, 10mM of Compound B was added to the 1mM ^{15}N- MMP-13:Compound A sample followed by pH readjustment.

NMR Data Collection: All spectra were recorded at 35°C on a Bruker AMX-2 600 spectrometer using a gradient enhanced triple-resonance $^{1}H/^{13}C/^{15}N$ probe. For spectra recorded in H_2O, water suppression was achieved with the WATERGATE sequence and water-flip back pulses (Piotto, *et al.*, J. Biomol. NMR 1992; Grzesiek and Bax, J. Am. Chem. Soc. 1993). Quadrature detection in the indirectly detected dimensions were recorded with States-TPPI hypercomplex phase increment (Marion, *et al.*, J. Magn. Reson. 1989). Spectra were collected with appropriate refocusing delays to allow for 0,0 or -90,180 phase correction.

The resonance assignments and bound conformation of Compound A in the MMP-1: Compound A complex were based on the 2D $^{12}C/^{12}C$-filtered NOESY (Petros, *et al.*, FEBS Lett. 1992; Gemmecker, *et al.*, J. Magn. Reson. 1992), 2D $^{12}C/^{12}C$-filtered TOCSY (Petros, *et al.*, FEBS Lett. 1992; Gemmecker, *et al.*, J. Magn. Reson. 1992) and $^{12}C/^{12}C$-filtered COSY experiments (Ikura and Bax, J. Am. Chem. Soc. 1992).

The assignments of the ^{1}H, ^{15}N, and ^{13}C resonances of MMP-13 in the MMP-13:Compound B complex were based on the previous assignments for the MMP-13:Compound A complex in combination with a minimal set of experiments: 2D ^{1}H-^{15}N HSQC, 3D ^{15}N- edited NOESY (Marion, *et al.* Biochemistry 1989; Zuiderweg and Fesik, Biochemistry 1989), CBCA(CO)NH (Grzesiek and Bax, J. Am. Chem. Soc. 1992), C(CO)NH (Grzesiek, *et al.*, J. Magn. Reson., Ser. B 1993), HNHA (Vuister and Bax, J. Am. Chem. Soc. 1993) and HNCA (Kay, *et al.*, J. Magn. Reson. 1990). The acquisition parameters for each of the experiments used in determining the solution structure of the MMP-13:Compound B complex were as reported previously (Moy, *et al.*, Biochemistry 1996).

The MMP-13:Compound B structure is based on observed NOEs from the 3D ^{15}N-edited NOESY (Marion, *et al.* Biochemistry 1989; Zuiderweg and Fesik, Biochemistry 1989) and 3D ^{13}C-edited/^{12}C-filtered NOESY (Vuister

and Bax, J. Am. Chem. Soc. 1993; Lee, *et al.*, FEBS Lett. 1994). The 3D ^{15}N-edited NOESY and 3D ^{13}C-edited/^{12}C-filtered NOESY experiments were collected with 100 msec and 110 msec mixing times, respectively.

Molecular Analysis and Design: The minimized models of Compound B and Compound D complexed to MMP-13 were prepared as previously described (Chen, *et al.*, J. Biomol. Struct. Dyn. 1995; Chen, *et al.*, Biochemistry (in press) 1998). Using molecular dynamics methods (Sybyl v6.4 from Tripos Inc), protein regions within 5 Å from Compound B were sampled along with the inhibitor, whereas everything else remained rigid during the simulations. Upon energy convergence, the last 50 frames from the final 100 picoseconds run was averaged and this averaged structure underwent a final minimization. The final protein-Compound B model appeared to have optimized possible polar and van der waals interactions. The identical procedure was applied to the complex of MMP-13 and Compound D. Since the two complexes used identical MMP-13 structures, the proteins were overlapped to depict the positions of the two inhibitors within the active site. Graphics analysis of the inhibitors showed that the methylene carbon of Compound B containing the 2HB1/2 protons (Figure 6) overlapped identically with the methoxy carbon from Compound D. This analysis indicated the optimal or minimal linkage length of connecting the benzofuran moiety to the methoxy region of Compound D. The final design scheme is shown in Figure 8A for the hybrid inhibitor. The homology model of MMP-9 was constructed using the COMPOSER program (Tripos INC, Sybyl v.6.4)

High-throughput Screening Analysis: Compound B was identified as an initial lead from the analysis of the MMP-13 high-throughput screen (HTS). A total of 58079 compounds were screened for their ability to inhibit MMP-13 enzymatic activity where 385 compounds were shown to have ≥ 40% inhibition at 10 μg/ml dosage. Compound B was shown to exhibit weak inhibition of MMP-13 (89% at the 10 μg/ml), but more intriguing was the observation of a complete

lack of activity against other MMPs (MMP-1, MMP-9 and TACE). The primary structure of Compound B along with the proton naming convention is shown in Figure 6.

The resulting HTS hits were further examined by cluster analysis. The hits were clustered based on structural similarities where the properties of these compounds were compared against the properties of the set of orally available drugs. The properties used to profile the HTS hits consists of: total number of non-hydrogen atoms, number of heteroatoms, number of hydrogen-bond donors and acceptors, calculated logP and molecular weight. This profile analysis provides an initial means to predict the likelihood that an HTS hit may have drug-like characteristics such as bioavailability and in-vivo stability. The profile of Compound B indicates that the compound has properties similar to orally available drugs suggesting that it would be an ideal candidate for optimization of its enzyme potency and selectivity.

A common feature of known MMP inhibitor structures is the presence of a Zn-chelator that plays a fundamental role in its activity. In most cases Zn chelation occurs from the presence of a hydroxamic acid in the structure of the small molecule. As apparent from the structure of Compound B, the compound does not contain an obvious substituent that would chelate Zn. Thus, the unique structure of Compound B suggested a potential novel mechanism for inhibition of MMP-13 further strengthening the choice of Compound B as an initial lead candidate. Therefore, the identification of Compound B as a candidate to optimize its activity and selectivity was based on three unique observations: its intrinsic MMP-13 selectivity, its structural profile similar to known bioavailable drugs and finally its apparent novel structure.

NMR Structure of the MMP-13 - Compound B Complex: The NMR binding studies provided critical information pertaining to the mechanism of Compound B inhibition of MMP-13 and the method for designing increase potency. The major question presented when Compound B was identified from HTS was its unknown MMP-13 binding site and its method for inducing MMP-13 inhibition.

Previous work on the NMR structure of MMP-13 complexed with Compound A and MMP-1 complexed with CGS-27023A provided the framework and methodology to analysis Compound B bound to MMP-13 (Moy, *et al.*, Biochemistry Submitted 1999; Moy, *et al.*, Biochemistry 1999).

The Compound B MMP-13 binding site was initially identified from chemical shift perturbation in the ^{1}H-^{15}N HSQC spectra. The observed perturbations were mapped onto a GRASP surface (not shown). It is apparent that the major effect of Compound B on the chemical shifts of MMP-13 occurs in the proximity of the S1' pocket suggesting that Compound B sits in this pocket. From the NMR and X-ray structures of MMP-13, it was determined that the S1' pocket for MMP-13 is very deep and linear in shape while nearly reaching the surface of the protein. In fact, a number of residues at the surface of MMP-13 near the base of the S1' pocket show significant chemical shift perturbation in the presence of Compound B. Since Compound B is a linear molecule, docking studies would place the inhibitor stretched throughout the linear S1' pocket of MMP-13. The only question remaining was whether to place the morpholine or the benzofuran moiety of Compound B at one end of the pocket, adjacent to the catalytic zinc or the opposite end, distant from the zinc atom. Property analysis of the enzymes S1' pocket depicts that the end adjacent to the zinc is relatively polar whereas the opposite end is hydrophobic. This analysis lead us to dock Compound B with the morpholine ring adjacent to the catalytic zinc atom with the benzofuran moiety siting in a hydrophobic pocket formed by L115, L136, F149 and P152 at the base of the S1' pocket. To further verify the proposed binding of Compound B in the S1' pocket of MMP-13, a simple competition experiment with Compound A was conducted. The ^{1}H-^{15}N HSQC experiment for the MMP-13:Compound B complex was collected in the presence of Compound A. The presence of Compound A displaced all of Compound B as evident by the distinct differences in the ^{1}H-^{15}N HSQC spectra which further suggests that both compounds bind in the S1' pocket.

The relative orientation and binding of Compound B with MMP-13 was further confirmed by the observation of intermolecular NOEs between

Compound B and MMP-13 from the 3D ^{13}C-edited/^{12}C-filtered NOESY experiment. The NOESY spectra was collected in the presence of a ten-fold excess of Compound B because of the weak affinity of Compound B with MMP-13. Nevertheless, a total of 16 NOEs were observed between Compound B and L81, L115, V116, Y141, T142 and Y143 which support the initial positioning of Compound B in the MMP-13 S1' pocket. An expanded 2D plane from the 3D ^{13}C-edited/^{12}C-filtered NOESY experiment (not shown) demonstrated examples of some key intermolecular NOEs between Compound B benzofuran group resonances and L115 δ and Compound B resonances proximal to the morpholine ring and L82 δ. The complex of Compound B with MMP-13 was subjected to energy refinement using the NMR results as constraints (Moy, *et al.*, Biochemistry 1999; Chen, *et al.*, J. Biomol. Struct. Dyn. 1995). The modeling results depict the morpholine oxygen forming a hydrogen bond with the backbone amide group of Leu-82 and the benzofuran group packs deep in the S1' pocket with the peptide bond linker portion forming hydrogen bonds with protein backbone groups. The complex shows no apparent interactions between the inhibitor and the catalytic zinc justifying the ligands micromolar potency.

Structures of MMP-1, MMP-9 and MMP-13: The recent NMR solution structures of MMP-1 and MMP-13 were used as starting points for molecular modeling and analysis (Moy, *et al.*, Biochemistry Submitted 1999; Moy, *et al.*, Biochemistry 1998; Moy, *et al.*, Biochemistry 1999). A homology model for MMP-9 was developed based on its strong homology to MMP-1 (54% identity around the catalytic domain). Based on the homology model, the catalytic site of MMP-9 is similar to the corresponding sites in MMP-1 and MMP-13. All three structures were used as starting points for analysis and synthetic design.

Comparative analysis of the MMP structures shows that residue positions 115 and 144, in addition to the length of the specificity loop, determines the size and shape of the S1' pockets. Alignment of the NMR structures for MMP-1 and MMP-13 shows that MMP-13 contains two additional

insertions in the specificity loop. The homology model of MMP-9 indicates no additional insertions so its length is identical to MMP-1.

Residue positions 115 and 144 are important in establishing the relative length of the S1' pockets for the MMPs where the larger the side chain at these positions results in a smaller S1' pocket. Since residue 115 is spatially closer to the catalytic zinc than residue 144, a larger side chain for residue 115 will have a greater impact on defining a smaller S1' pocket compared to residue 144. MMP-1 has the largest side chain at position 115, thus its S1' pocket is the smallest. MMP-9 has an Arg at position 144 resulting in its S1' pocket being longer compared to MMP-1. Conversely, MMP-13 has short side chains at both positions 115 and 144. The short side chains combined with an increased length of its specificity loop result in MMP-13 having the largest S1' pocket. To summarize, the size of the MMP S1' pockets are as follows: MMP-13 > MMP-9 > MMP-1 where this structural feature plays a critical role in the design strategy for developing a potent and specific MMP-13 inhibitor.

Design Strategy: A strategy utilizing NMR and molecular modeling was applied towards the design and synthesis of an MMP-13 selective inhibitor lead. The basic approach behind the design strategy is to optimize the affinity of the chemical lead Compound B while maintaining its inherent MMP-13 selectivity. This can be achieved by taking advantage of the distinct structural feature of MMP-13, its deep linear S1' pocket, while combining overlapping structural features of Compound B with other potent inhibitors. Compound C is an example of a potent and selective inhibitor for MMP-9 and MMP-13 (See Table 2). Based on the NMR solution structure of MMP-13 complexed with Compound A (Figure 4), structurally similar inhibitors were positioned into the active site of MMP-13.

Figure 7 shows the critical regions of Compound C, which can be broken down into two components, Compound D which represents the zinc chelating portion of the compound that contributes to the binding potency and the toluene group (1A) which contributes to enhanced ligand selectivity against

MMP-1. The strategy was to design a new inhibitor based on replacing the toluene group (1A) with a component of Compound B critical for binding within the extended S1' pocket of MMP-13. The overlay of the NMR solution structure for Compound B with the model for Compound D is shown in Figure 8B. The close similarity between the positioning of the two structures made it readily apparent that it would be possible to generate a hybrid of the two structures combining the potent Compound D with the selective component of Compound B (Figure 8A). These results were then used to design the proposed hybrid inhibitor Compound E. The assay data in Table 2 clearly shows that the new inhibitor, Compound E, has better potency compared to Compound C in addition to improved selectivity towards MMP-13. Thus, the combination of NMR spectroscopy with molecular modeling techniques resulted in the design of a novel, potent and selective MMP-13 inhibitor (Compound E) which has an IC50 of 17 nM for MMP-13 and showed >5800, 56 and >500 fold selectivity against MMP-1, MMP-9 and TACE, respectively. To the best of our knowledge, this represents the first example of a potent MMP-13 inhibitor that has been shown to be selective against MMP-9.

Table 2 - IC50 and Selectivity Data

Compound	MMP-1	MMP-9	MMP-13	TACE	S-1[a]	S-9[a]	S-TACE[a]
C	750nM	46nM	75nM	470nM	10.0x	0.6x	6.3x
D	82nM	21nM	15nM	240nM	5.5x	1.4x	16x
E	NA	945nM	17nM	19%	>5800x	56x	>500x
F	1025nM	71nM	301nM	664nM	3.4x	0.2x	2.2x

[a] Selectivity data presented as a ratio of the MMP or TACE IC50 with MMP-13

Example 4

The X-ray crystal structure of the MMP-13:Compound A complex was determined using the following procedure:

Gene/expression system/production: The cDNA coding for human MMP-13 proenzyme had 85 residues of the PRO domain, followed by 165 residues of the catalytic domain (CAT). The gene was carried on a pET-21a expression plasmid, under the control of a bacteriophage T7 promoter. The expression host was *Escherichia coli* BL21(DE3), which had a chromosomal copy of T7 RNA polymerase under *lac* control. Cells were grown in nutrient broth, and synthesis of PRO-CAT was induced by isopropyl-β-thiogalactoside. The protein accumulated to 5-10% of total cellular protein, essentially all of which was aggregated into inclusion bodies.

For potential MAD experiments, the plasmid was transferred into a methionine auxotroph host. PRO-CAT with selenomethionine substitution was produced by induction in a defined medium, with methionine replaced by selenomethionine.

Purification and refolding of PRO-CAT: Frozen cells were disrupted mechanically, and inclusion bodies were isolated by centrifugation. PRO-CAT was solubilized with urea containing dithiothreitol to disrupt any disulfide bridges. PRO-CAT was partially purified by anion-exchange chromatography, in urea, on Q Sepharose. The protein was diluted to about 400 μg/ml in a solution of sodium chloride, calcium chloride, and zinc acetate, buffered with tricine-HCl. Refolding proceeded over 3-4 days, during dialysis, with multiple buffer changes. PRO-CAT was then concentrated for activation and release of CAT.

Activation of PRO-CAT: The presently-accepted view of MMPs holds that the proenzyme form is maintained in an inactive state through the coordination of one cysteine from the PRO domain into the active-site zinc. If this cysteine is

displaced, the enzyme becomes active. In our protocol, aminophenyl mercuric acetate was added to the protein solution to form a mercurial adduct with the cysteine. Progress of activation was monitored by SDS polyacrylamide gel eletrophoresis. Results indicated that the CAT domain accumulated and the PRO domain was degraded to small peptides.

Purification of MMP-13 (CAT) – Size Exclusion: Following activation and PRO cleavage, MMP-13 was isolated by size-exclusion chromatography through SuperDex 75 in a solution of sodium chloride, calcium chloride, and zinc acetate, buffered with tris-HCl.

Purification of MMP-13 – Affinity: MMP-13 was further purified by affinity chromatography on an immobilized hydroxamate inhibitor. The affinity matrix was prepared by coupling an hydroxamate inhibitor to Sepharose through the amino group of the piperazine ring. MMP-13 can be absorbed to the matrix and desorbed by displacement using another inhibitor of choice.

Characterization of MMP-13: Protein preparations for crystallization trials were validated by several techniques. Routinely, SDS-PAGE showed a predominant species whose migration was consistent with a molecular weight of around 19,000. MALDITOF mass spectroscopy demonstrates a single species consistent with the expected size of 18,588 amu. (MMP-13 prepared with selenomethionine showed essentially complete replacement). N-terminal sequencing demonstrated that the protein begins with YNVF, as expected for correct cleavage between PRO and CAT. Retention volume in analytical size-exclusion chromatography was consistent with a monomeric protein: no detectable aggregation was observed. The final protein was enzymatically active on a fluorogenic peptide substrate, and degraded denatured collagen.

Crystallization of MMP-13 complex with Compound A: The MMP-13 protein solution was buffered with 10 mM tris-HCL buffer, pH 7.5, and 0.25 M NaCl.

The concentration of protein used for crystallization was 20.0 mg/ml. The inhibitor solution was added to a protein solution with a mole ratio (protein:inhibitor) of 1:2, and was mixed for more than 1 hour.

Crystallization conditions were screened by the hanging-drop vapor diffusion method (Mcpherson, A., Methods Biochem. Anal. 1976). A successful procedure for growing crystals of this complex at room temperature was identified, and crystals were obtained. Specifically, a solution was prepared from 3 µl of protein solution and 3 µl of precipitant solution, which consisted of 26% PEG4000, 0.1 M ammonium sulfate, and 0.1 M sodium chloride. A drop of this solution was suspended on a microscope coverslip glass which had been coated with silicone to prevent drop spreading. The reservoir solutions consisted of 0.6 ml precipitant solution. Equilibration was performed at room temperature by vapor diffusion. Crystals began appearing after three days. After two weeks, these crystals stopped growing. The X-ray data which have been processed show that the MMP-13 complex was crystallized in two forms. One crystal form is C-centered orthorhombic; it belonged to space group C2221, and had a cell dimension of a=36.3 Å, b=134.4 Å, and c=134.8 Å. This crystal had high mosaicity; therefore, it would be of little use when working on the structure of the complex. The second crystal form is primitive orthorhombic, from space group P21212, with a cell constant of a=108.3 Å, b=79.8 Å, and c=36.1 Å. This crystal had low mosaicity, but it was very small in most cases.

In order to obtain a big single crystal for X-ray data collections, the seeding technique (Thaller, C., et al., J. Mol. Biol. 1981) was applied. This was accomplished by using both the microseeding and the macroseeding methods. Small seed crystals were transferred to a 20% PEG4000 precipitant solution on a depression slide. A single washed crystal was injected into a hanging-drop solution, which was composed of 3 µl of MMP-13 complex solution and 3 µl of precipitant solution. The reservoir solutions consisted of 0.6 ml precipitant solution at pH 8.0. This procedure successfully produced bigger crystals with a maximum edge dimension of up to 0.35 x 0.1 x 0.1 mm^3. These crystals diffracted X-ray at a resolution of 2.0 Å.

X-Ray Data Collection: X-ray diffraction data from 30.0-2.0 Å resolution for the MMP-13:Compound A complex crystal (P21212 form) was collected by using an RAXIS IIc Image Plate area detector which used graphite monochromatic CuKα radiation from a Rigaku RU200 rotating anode generator (operating at 50 kV, 100 mA) at a low temperature of 100 K. The oscillation angle for each plate was 1 degree, and exposure time was 20 minutes per 'image'. The processing of X-ray diffraction data was accomplished using the HKL programs (Otwinowski, Z. and Minor, W., Methods in Enzymology 276:307-26). The R-merges for full and partial reflections were 4.0% and 6.04% respectively. 18,782 unique reflections (81% complete at 2.0 Å resolutions) were collected.

Structure Determination and Refinement: The MMP-13 complex crystal structure has been determined by a combination of crystallographic modeling and the Molecular Replacement method using models of MMP-13 derived from the MMP-1 and MMP-8 structures. The homology between MMP-13 and MMP-8 is 56% by sequence, and at least 70% by structure. Crystals of the MMP-13 complex have two molecules in the asymmetric unit, *i.e.*, the unit is a dimer. Conventional molecular replacement was not effective for determination of this dimer structure by using a monomer model. There are two reasons for this: (1) the high symmetry of the crystal structure; and (2) the conformations and the configurations of the side chain and the main chain in flexible loops of MMP-13 and MMP-8.

Firstly, the crystal structure of the MMP-13 complex is highly symmetrical. The P21212 crystal has four symmetry operations, and there are eight molecules in a unit cell. A second crystal form, belonging to space group C222, and having eight symmetry operations in a unit cell, has been identified. In this crystal, there are 16 monomers per cell in the dimer structure, and 32 monomers per cell in the tetramer structure. Therefore, the rotation search and especial translation search become more difficult. Secondly, even though the MMP family's catalytic domain structure is highly conserved, the conformations and the configurations of the side chain and the main chain in flexible loops of

MMP-13 and MMP-8 may not be the same. In particular, the similarity between the two structures may not be sufficient to permit the determination of the dimer structure using a monomer as the searching model.

Many attempts at a rotation and translation search were made by using the X-ray data and models of either a monomer of MMP-8 or a dimer of MMP-1. Some rotation solutions were obtained, but no final translation solution has been found by using the monomer model. Accordingly, to determine this structure, it was proposed that a dimer model be constructed first; the molecular replacement method was then applied to solve the structure.

The key idea of this proposal was crystal packing. To construct a dimer, the orientations of each monomer were determined on the basis of a rotation search. The positions of each monomer were located on the basis of the molecular packing in unit cell. Many dimer models have been constructed and applied as the 'model' for searching the rotation and translation using program AMORE (Collaborative Computational Project, Number 4 (CCP4) (1994), Acta Cryst. D50:760-763). One dimer model was found to be correct, and finally resulted in the MMP-13 3-D crystal structure using the molecular replacement method. The MMP-13 complex structure was confirmed by observing the most important and significant fact that the positions of the two zinc ions and the two calcium ions could be identified from the difference (Fo-Fc) maps with five-sigma cut, where Fo was observed structure factor and Fc was the calculated structure factor of the dimer model without zinc and calcium atoms.

These ions were located in the exact positions where they were observed in other MMP family members. The molecule fits the (2Fo-Fc) electron densities very well, both in main chain and in side chain. The molecule fits the 2Fo-Fc electron density quite well. All of these MMP molecules are conserved in the core structure region, especially the position of the central helix and the catalytic zinc. The MMP-13 dimer structure was further confirmed by applying the molecular replacement programs XPLOR (Brünger, A.T., XPLOR Version 3.1 Manual, Yale University, New Haven CT) and MERLOT (Fitzgerald,

P., MERLOT, version 2.4 (Nov. 10, 1991). All of them worked very well, and produced results which were in agreement with the MMP-13 structure.

Structure Refinement: The structure refinement was carried out by the program XPLOR. The initial dimer model included 320 amino acid residues without zinc and calcium ions. The dimer model was refined against 2.0 Å X-ray data, collected on an RAXIS IIc area detector at a temperature of 100 K. The progress of the refinement was evaluated from the quality of the protein molecular conformations and the electron density maps, and the values of the crystallographic R-factor. The initial R-factor was 52%. After rigid-body minimization, conjugated-gradient minimization, a heating stage, a slow-cooling stage in the range from 4000K to 300K, energy minimization, B-factor refinement, and positional refinement, the R-factor lowered to 0.32. Electron-density maps with coefficients of (2Fo-Fc) and (Fo-Fc), as well as the phases, were calculated. The difference map shows four zinc ions and four calcium ions in the dimer structure with five-sigma cut. Some side chain loops and a few main loops were rebuilt on the interactive graphics system. The rebuilt dimer plus the zinc and calcium ions, as the new model, was refined. The R-factor was down to 26.6%. At this stage, a model of inhibitor Compound A was positioned in the active-site region based on the difference electron density.

The complex structure was refined by repeating the above steps, with the R-factor down to 20%. The water molecules were modeled as oxygen atoms. Their initial positions were located by searching the peaks in the (Fo-Fc) difference maps. These positions were then checked by calculating the distance between 'water' and the oxygen and nitrogen of the protein. Together with the protein (complex) atoms, these 'water' molecules were refined against the X-ray data. Once the temperature factor of water was higher than 50, this water was omitted. 120 water molecules near the protein were found, and five water molecules were identified in the active site of each monomer. The (2Fo-Fc) maps were used to adjust the solvent model and to aid in the placement of new solvent molecules, as well as to check and correct the whole model. The r.m.s.

deviations of Cα atoms for bond angles and bond distances from ideal geometry were 1.6° and 0.012 Å. The final crystallographic R-factor was 22%, at a resolution of 2.0 Å.

All publications mentioned herein above, whether to issued patents, pending applications, published articles, protein structure deposits, or otherwise, are hereby incorporated by reference in their entirety. While the foregoing invention has been described in some detail for purposes of clarity and understanding, it will be appreciated by one skilled in the art from a reading of the disclosure that various changes in form and detail can be made without departing from the true scope of the invention in the appended claims.

What is claimed is:

1. A solution comprising a biologically active catalytic fragment of human collagenase-3 (MMP-13) complexed with N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-methyl-benzamide ("Compound A").

2. The solution of Claim 1, wherein the catalytic fragment of MMP-13 comprises the amino acid residues of Figure 1.

3. The solution of Claim 2, comprising 1 mM MMP-13 complexed with Compound A in a 1:1 molar ratio, in a buffer comprising 10mM deuterated Tris-Base, 100mM NaCl, 5mM $CaCl_2$, 0.1mM $ZnCl_2$, 2mM NaN_3, and 10 mM deuterated DTT in either 90% H_2O/10% D_2O or 100% D_2O.

4. The solution of Claim 3, wherein the MMP-13 is either ^{15}N enriched or ^{15}N,^{13}C enriched.

5. The solution of Claim 1, wherein the secondary structure of the catalytic fragment of MMP-13 comprises three alpha helices and a mixed parallel and anti-parallel beta sheet comprising five beta strands.

6. The solution of Claim 5, wherein the alpha helices and beta strands are configured in the order β_I, α_A, β_{II}, β_{III}, β_{IV}, β_V, α_B, and α_C.

7. The solution of Claim 6, wherein the three alpha helices correspond to residues 28-44 (α_A), 112-123 (α_B) and 153-163 (α_C) of Figure 1, and the five beta strands correspond to residues 83-86 (β_I), 95-100 (β_{II}), 59-66 (β_{III}), 14-20 (β_{IV}), and 49-53 (β_V) of Figure 1.

8. A crystallized catalytic fragment of MMP-13 complexed with N-Hydroxy-2-[(4-methoxy-benzenesulfonyl)-pyridin-3-ylmethyl-amino]-3-

methyl-benzamide ("Compound A").

9. The crystallized complex of Claim 8, wherein the catalytic fragment of MMP-13 comprises the amino acid residues of Figure 1.

10. The crystallized complex of Claim 9, characterized as being in orthorhombic form with space group P21212, and having unit cell parameters of a=108.3Å, b=79.8Å, and c=36.1Å.

11. The crystallized complex of Claim 10, further characterized as consisting of two molecules of MMP-13:Compound A complex in the asymmetric unit.

12. The crystallized complex of Claim 11, wherein the secondary structure of the catalytic fragment of MMP-13 comprises three alpha helices and a mixed parallel and anti-parallel beta sheet comprising five beta strands.

13. The crystallized complex of Claim 12, wherein the alpha helices and beta strands are configured in the order β_I, α_A, β_{II}, β_{III}, β_{IV}, β_V, α_B, and α_C.

14. The crystallized complex of Claim 13, wherein the three alpha helices correspond to residues 28-44 (α_A), 112-123 (α_B) and 153-163 (α_C) of Figure 1, and the five beta strands correspond to residues 83-86 (β_I), 95-100 (β_{II}), 59-66 (β_{III}), 14-20 (β_{IV}), and 49-53 (β_V) of Figure 1.

15. An active site of MMP-13, characterized by a catalytic zinc, a beta strand, a Ca^{2+} binding loop, an alpha helix, and a random coil region.

16. The active site of Claim 15, wherein the beta strand comprises residues N14, L15, T16, Y17, R18, I19, and V20 according to Figure 1, the Ca^{2+} binding loop comprises residues F75, D76, G77, P78, and S79 according to Figure 1, the alpha helix comprises residues N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, and H123 according to Figure 1, and the random coil region comprises residues P139, I140, and Y141 according to Figure 1.

17. The active site of Claim 16, wherein said active site comprises the relative structural coordinates of the catalytic zinc and amino acid residues N14, L15, T16, Y17, R18, I19, V20, F75, D76, G77, P78, S79, N112, L113, F114, L115, V116, A117, A118, H119, E120, F121, G122, H123, P139, I140, and Y141 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å.

18. The active site of Claim 17, further comprising the relative structural coordinates of amino acid residues G80, L81, L82, A83, H84, A85, K109, G110, Y111, S124, L125, G126, L127, D128, H129, S130, K131, D132, P133, G134, A135, L136, M137, F138, T142, Y143, T144, and G145 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å.

19. The active site of Claim 18, further comprising the relative structural coordinates of amino acid residues F149 and P152 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å.

20. An active site of MMP-13 comprising the relative structural coordinates of a catalytic zinc and amino acid residues L81, L82, L115, V116, H119, L136 and I140 according to the solution or crystal coordinates of Figures 4 or 5, respectively, in each case, ± a root mean square deviation from the catalytic zinc and the conserved backbone atoms of said amino acids of not more than 1.5Å.

21. A method for identifying a potential inhibitor or activator of MMP-13, comprising the steps of:

(a) using a three dimensional structure of MMP-13 as defined by the relative structural coordinates of amino acids encoding MMP-13 according to Figures 4 or 5, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 1.5Å;

(b) employing said three-dimensional structure to design or select a potential inhibitor or activator; and

(c) synthesizing or obtaining said potential inhibitor or activator.

22. The method according to Claim 21, wherein the potential inhibitor is designed de novo.

23. The method according to Claim 21, wherein the potential inhibitor is designed from a known inhibitor.

24. The method of Claim 22, further comprising the step of contacting the potential inhibitor with MMP-13 in the presence of a substrate to determine the ability of the potential inhibitor to inhibit MMP-13.

25. The method of Claim 23, further comprising the step of contacting the potential inhibitor with MMP-13 in the presence of a substrate to determine the ability of the potential inhibitor to inhibit MMP-13.

26. The method according to Claim 21, wherein the step of employing the three dimensional structure to design or select the potential inhibitor comprises the steps of:

(a) identifying chemical entities or fragments capable of associating with MMP-13; and

(b) assembling the identified chemical entities or fragments into a single molecule to provide the structure of the potential inhibitor.

27. The method according to Claim 26, wherein the potential inhibitor is designed de novo.

28. The method according to Claim 26, wherein the potential inhibitor is designed from a known inhibitor.

29. The method of Claim 27, further comprising the step of contacting the potential inhibitor with MMP-13 in the presence of a substrate to determine the ability of the potential inhibitor to inhibit MMP-13.

30. The method of Claim 28, further comprising the step of contacting the potential inhibitor with MMP-13 in the presence of a substrate to determine the ability of the potential inhibitor to inhibit MMP-13.

31. An inhibitor identified or designed by the method of Claim 21.

32. An inhibitor identified or designed by the method of Claim 26.

YNVFP	RTLKW	SKMNL	TYRIV	NYTPD
5	10	15	20	25
MTHSE	VEKAF	KKAFK	VWSDV	TPLNF
30	35	40	45	50
TRLHD	GIADI	MISFG	IKEHG	DFYPF
55	60	65	70	75
DGPSG	LLAHA	FPPGP	NYGGD	AHFDD
80	85	90	95	100
DETWT	SSSKG	YNLFL	VAAHE	FGHSL
105	110	115	120	125
GLDHS	KDPGA	LMFPI	YTYTG	KSHFM
130	135	140	145	150
LPDDD	VQGIQ	SLYG		
155	160	164		

FIG. 1

Sequence 1: MMP-13
Sequence 2: MMP-1
Identity score: 58.9 %

```
VGEYNVFPRTLKWSKMNLTYRIVNYTPDMTHSEVEKAFKKAFKVWSDVTPLNFTRLHDGIADIMISFGIKEHGDFYPFDG
LTEGN  PR   WEQTHLTYRIENYTPDLPRADVDHAIEKAFQLWSNVTPLTFTKVSEGQADIMISFVRGDHRDNSPFDG

PSGLLAHAFPPGPNYGGDAHFDDDETWTS          SSKGYNLF          LVAAHEFGHSLGLDHSKDPGALMF
PIYTYTGKSHFMLPDDDVQ
PGGNLAHAFQPGPGIGGDAHFDEDERWTNNFREYNLHRVAAHELGHSLGLS HST DIGALMYPSYTFSGDVQ   LAQDD
ID
                                                                              ###

GIQSLYGPGDEDPN
GIQAIYGRSQ
```

FIG. 2A

Sequence 1: MMP-13
Sequence 2: MMP-8
Identity score: 61.4 %

```
VGEYNVFPRTLKWSKMNLTYRIVNYT PDMTH S EVEKAFKKAFKVWSDVTPLNFTRLHDGIADIMISFGIKEHGDFYPFDG
          NPKWER T NLTYRIRNYTP QLSEA  EVERAI KDAFEL WSVASPLI
FTRISQGEADINIAFYQRDHGDNSPFDG
                          ••

PSGLLAHAFPPGPNYGGDAHFDDDETWTSSSKGYNLFLVAAHEFGHSLGLDHSKDPGALMF PIYTYTGKSHFMLPDDDVQ
PNGILAHAFQPGQGIGGDAHFDAEETWTNTSANYNLFLVAA HEFGHSLGLAHSSDPGALMYPNYAF RETSNYSLPQDD ID
                                                                  ###

GIQSLYGPGDEDPN
GIQAIYG
```

FIG. 2B

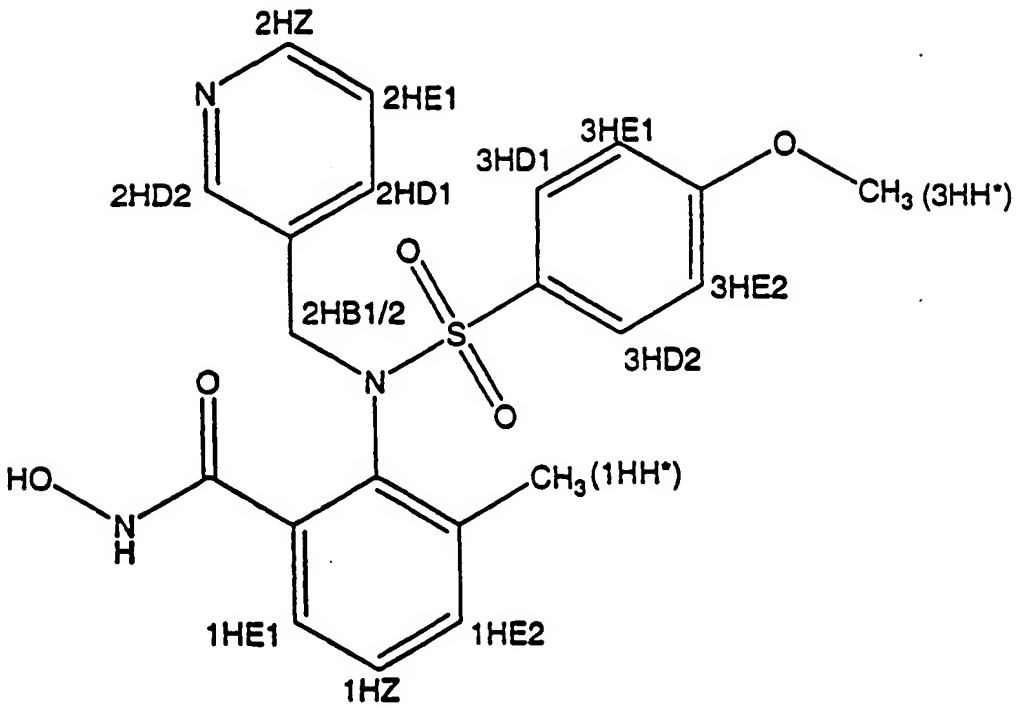

2HZ
N
2HE1
2HD2
2HD1
3HE1
3HD1
O
CH3 (3HH*)
3HE2
3HD2
O
2HB1/2
S
O
N
O
HO
N
H
CH3 (1HH*)
1HE1
1HE2
1HZ

FIG. 3

		Atom Type	Res.		X	Y	Z		
ATOM	1	N	THR	7	-12.675	-13.911	-8.815	1.00	0.83
ATOM	2	HN	THR	7	-12.001	-14.254	-8.192	1.00	1.22
ATOM	3	CA	THR	7	-14.063	-13.649	-8.340	1.00	0.63
ATOM	4	HA	THR	7	-14.744	-14.330	-8.830	1.00	0.73
ATOM	5	CB	THR	7	-14.132	-13.858	-6.825	1.00	0.61
ATOM	6	HB	THR	7	-13.473	-13.158	-6.335	1.00	0.66
ATOM	7	OG1	THR	7	-13.730	-15.185	-6.514	1.00	0.71
ATOM	8	HG1	THR	7	-13.721	-15.690	-7.330	1.00	1.07
ATOM	9	CG2	THR	7	-15.564	-13.628	-6.336	1.00	0.67
ATOM	10	HG21	THR	7	-15.712	-12.577	-6.139	1.00	1.14
ATOM	11	HG22	THR	7	-15.728	-14.191	-5.429	1.00	1.32
ATOM	12	HG23	THR	7	-16.261	-13.955	-7.093	1.00	1.23
ATOM	13	C	THR	7	-14.451	-12.208	-8.678	1.00	0.52
ATOM	14	O	THR	7	-15.416	-11.962	-9.374	1.00	0.65
ATOM	15	N	LEU	8	-13.704	-11.254	-8.195	1.00	0.47
ATOM	16	HN	LEU	8	-12.927	-11.473	-7.639	1.00	0.61
ATOM	17	CA	LEU	8	-14.027	-9.831	-8.495	1.00	0.42
ATOM	18	HA	LEU	8	-15.098	-9.715	-8.575	1.00	0.43
ATOM	19	CB	LEU	8	-13.495	-8.937	-7.370	1.00	0.52
ATOM	20	HB1	LEU	8	-13.721	-7.905	-7.591	1.00	0.54
ATOM	21	HB2	LEU	8	-12.424	-9.060	-7.292	1.00	0.58
ATOM	22	CG	LEU	8	-14.151	-9.331	-6.042	1.00	0.60
ATOM	23	HG	LEU	8	-13.958	-10.376	-5.844	1.00	0.60
ATOM	24	CD1	LEU	8	-13.566	-8.484	-4.910	1.00	0.74
ATOM	25	HD11	LEU	8	-13.899	-8.875	-3.960	1.00	1.22
ATOM	26	HD12	LEU	8	-13.900	-7.462	-5.016	1.00	1.26
ATOM	27	HD13	LEU	8	-12.488	-8.518	-4.956	1.00	1.31
ATOM	28	CD2	LEU	8	-15.664	-9.096	-6.117	1.00	0.61
ATOM	29	HD21	LEU	8	-15.871	-8.278	-6.791	1.00	1.13
ATOM	30	HD22	LEU	8	-16.040	-8.856	-5.134	1.00	1.18
ATOM	31	HD23	LEU	8	-16.149	-9.991	-6.478	1.00	1.26
ATOM	32	C	LEU	8	-13.374	-9.438	-9.822	1.00	0.40
ATOM	33	O	LEU	8	-12.218	-9.722	-10.064	1.00	0.45
ATOM	34	N	LYS	9	-14.109	-8.795	-10.687	1.00	0.36
ATOM	35	HN	LYS	9	-15.042	-8.581	-10.474	1.00	0.36
ATOM	36	CA	LYS	9	-13.536	-8.393	-12.002	1.00	0.37
ATOM	37	HA	LYS	9	-12.521	-8.050	-11.862	1.00	0.39
ATOM	38	CB	LYS	9	-13.539	-9.599	-12.944	1.00	0.50
ATOM	39	HB1	LYS	9	-12.851	-10.344	-12.573	1.00	0.60

FIG. 4

ATOM	40	HB2	LYS	9	-13.233	-9.286	-13.932	1.00	0.48
ATOM	41	CG	LYS	9	-14.948	-10.193	-13.007	1.00	0.60
ATOM	42	HG1	LYS	9	-15.632	-9.455	-13.398	1.00	0.66
ATOM	43	HG2	LYS	9	-15.260	-10.482	-12.014	1.00	0.78
ATOM	44	CD	LYS	9	-14.951	-11.421	-13.921	1.00	0.94
ATOM	45	HD1	LYS	9	-13.944	-11.794	-14.033	1.00	1.57
ATOM	46	HD2	LYS	9	-15.344	-11.147	-14.889	1.00	1.62
ATOM	47	CE	LYS	9	-15.829	-12.511	-13.303	1.00	0.57
ATOM	48	HE1	LYS	9	-16.776	-12.086	-13.007	1.00	1.15
ATOM	49	HE2	LYS	9	-15.333	-12.924	-12.437	1.00	1.10
ATOM	50	NZ	LYS	9	-16.060	-13.591	-14.304	1.00	1.61
ATOM	51	HZ1	LYS	9	-15.181	-14.127	-14.445	1.00	2.14
ATOM	52	HZ2	LYS	9	-16.358	-13.168	-15.207	1.00	2.13
ATOM	53	HZ3	LYS	9	-16.802	-14.231	-13.959	1.00	2.14
ATOM	54	C	LYS	9	-14.377	-7.265	-12.605	1.00	0.32
ATOM	55	O	LYS	9	-15.493	-7.021	-12.191	1.00	0.34
ATOM	56	N	TRP	10	-13.850	-6.571	-13.577	1.00	0.31
ATOM	57	HN	TRP	10	-12.947	-6.781	-13.895	1.00	0.33
ATOM	58	CA	TRP	10	-14.618	-5.456	-14.201	1.00	0.30
ATOM	59	HA	TRP	10	-15.030	-4.826	-13.427	1.00	0.29
ATOM	60	CB	TRP	10	-13.684	-4.630	-15.088	1.00	0.29
ATOM	61	HB1	TRP	10	-14.264	-3.917	-15.655	1.00	0.32
ATOM	62	HB2	TRP	10	-13.157	-5.286	-15.765	1.00	0.33
ATOM	63	CG	TRP	10	-12.699	-3.901	-14.230	1.00	0.25
ATOM	64	CD1	TRP	10	-11.516	-4.405	-13.812	1.00	0.30
ATOM	65	HD1	TRP	10	-11.137	-5.390	-14.040	1.00	0.37
ATOM	66	CD2	TRP	10	-12.786	-2.553	-13.683	1.00	0.21
ATOM	67	NE1	TRP	10	-10.872	-3.454	-13.042	1.00	0.30
ATOM	68	HE1	TRP	10	-9.996	-3.569	-12.617	1.00	0.36
ATOM	69	CE2	TRP	10	-11.614	-2.295	-12.934	1.00	0.23
ATOM	70	CE3	TRP	10	-13.758	-1.538	-13.763	1.00	0.24
ATOM	71	HE3	TRP	10	-14.663	-1.706	-14.328	1.00	0.29
ATOM	72	CZ2	TRP	10	-11.412	-1.075	-12.287	1.00	0.22
ATOM	73	HZ2	TRP	10	-10.509	-0.903	-11.720	1.00	0.27
ATOM	74	CZ3	TRP	10	-13.558	-0.309	-13.113	1.00	0.25
ATOM	75	HZ3	TRP	10	-14.310	0.463	-13.181	1.00	0.32
ATOM	76	CH2	TRP	10	-12.387	-0.078	-12.376	1.00	0.23
ATOM	77	HH2	TRP	10	-12.238	0.870	-11.879	1.00	0.26
ATOM	78	C	TRP	10	-15.755	-6.031	-15.050	1.00	0.39
ATOM	79	O	TRP	10	-15.641	-7.098	-15.620	1.00	0.48
ATOM	80	N	SER	11	-16.855	-5.332	-15.132	1.00	0.43
ATOM	81	HN	SER	11	-16.927	-4.476	-14.660	1.00	0.44
ATOM	82	CA	SER	11	-18.006	-5.835	-15.936	1.00	0.52
ATOM	83	HA	SER	11	-18.003	-6.915	-15.930	1.00	0.59
ATOM	84	CB	SER	11	-19.313	-5.330	-15.325	1.00	0.64
ATOM	85	HB1	SER	11	-19.120	-4.425	-14.763	1.00	1.16
ATOM	86	HB2	SER	11	-19.718	-6.079	-14.666	1.00	1.20
ATOM	87	OG	SER	11	-20.246	-5.067	-16.365	1.00	1.39
ATOM	88	HG	SER	11	-19.821	-4.495	-17.008	1.00	1.92
ATOM	89	C	SER	11	-17.893	-5.335	-17.379	1.00	0.47
ATOM	90	O	SER	11	-18.785	-5.528	-18.181	1.00	0.60
ATOM	91	N	LYS	12	-16.808	-4.692	-17.715	1.00	0.42
ATOM	92	HN	LYS	12	-16.101	-4.543	-17.053	1.00	0.51
ATOM	93	CA	LYS	12	-16.646	-4.178	-19.107	1.00	0.41
ATOM	94	HA	LYS	12	-17.243	-4.775	-19.781	1.00	0.47
ATOM	95	CB	LYS	12	-17.116	-2.722	-19.167	1.00	0.43
ATOM	96	HB1	LYS	12	-18.168	-2.674	-18.926	1.00	0.50
ATOM	97	HB2	LYS	12	-16.957	-2.334	-20.163	1.00	0.46
ATOM	98	CG	LYS	12	-16.327	-1.882	-18.160	1.00	0.41
ATOM	99	HG1	LYS	12	-15.275	-1.922	-18.401	1.00	0.37
ATOM	100	HG2	LYS	12	-16.484	-2.272	-17.164	1.00	0.42
ATOM	101	CD	LYS	12	-16.805	-0.430	-18.223	1.00	0.50
ATOM	102	HD1	LYS	12	-17.856	-0.386	-17.981	1.00	0.56
ATOM	103	HD2	LYS	12	-16.648	-0.044	-19.220	1.00	0.65
ATOM	104	CE	LYS	12	-16.018	0.412	-17.218	1.00	0.61
ATOM	105	HE1	LYS	12	-15.054	0.665	-17.636	1.00	1.15
ATOM	106	HE2	LYS	12	-15.879	-0.151	-16.307	1.00	1.16
ATOM	107	NZ	LYS	12	-16.773	1.661	-16.920	1.00	1.39
ATOM	108	HZ1	LYS	12	-16.498	2.018	-15.983	1.00	1.90
ATOM	109	HZ2	LYS	12	-17.794	1.458	-16.927	1.00	1.87
ATOM	110	HZ3	LYS	12	-16.556	2.379	-17.640	1.00	1.97
ATOM	111	C	LYS	12	-15.175	-4.269	-19.521	1.00	0.36
ATOM	112	O	LYS	12	-14.284	-4.250	-18.695	1.00	0.34
ATOM	113	N	MET	13	-14.917	-4.380	-20.796	1.00	0.37
ATOM	114	HN	MET	13	-15.652	-4.402	-21.443	1.00	0.40
ATOM	115	CA	MET	13	-13.506	-4.487	-21.269	1.00	0.38
ATOM	116	HA	MET	13	-12.910	-4.964	-20.506	1.00	0.39

ATOM	117	CB	MET	13	-13.469	-5.332	-22.543	1.00	0.46
ATOM	118	HB1	MET	13	-12.523	-5.189	-23.043	1.00	0.53
ATOM	119	HB2	MET	13	-14.273	-5.031	-23.199	1.00	0.42
ATOM	120	CG	MET	13	-13.632	-6.809	-22.178	1.00	0.64
ATOM	121	HG1	MET	13	-12.857	-7.097	-21.483	1.00	1.26
ATOM	122	HG2	MET	13	-13.556	-7.411	-23.071	1.00	1.37
ATOM	123	SD	MET	13	-15.252	-7.067	-21.414	1.00	1.22
ATOM	124	CE	MET	13	-14.663	-7.870	-19.903	1.00	0.57
ATOM	125	HE1	MET	13	-14.020	-7.189	-19.362	1.00	1.16
ATOM	126	HE2	MET	13	-14.107	-8.758	-20.158	1.00	1.09
ATOM	127	HE3	MET	13	-15.508	-8.141	-19.286	1.00	1.20
ATOM	128	C	MET	13	-12.936	-3.095	-21.560	1.00	0.32
ATOM	129	O	MET	13	-11.793	-2.957	-21.948	1.00	0.35
ATOM	130	N	ASN	14	-13.718	-2.064	-21.371	1.00	0.28
ATOM	131	HN	ASN	14	-14.635	-2.199	-21.052	1.00	0.29
ATOM	132	CA	ASN	14	-13.217	-0.681	-21.631	1.00	0.26
ATOM	133	HA	ASN	14	-12.359	-0.725	-22.286	1.00	0.29
ATOM	134	CB	ASN	14	-14.319	0.148	-22.297	1.00	0.30
ATOM	135	HB1	ASN	14	-14.025	1.186	-22.318	1.00	0.31
ATOM	136	HB2	ASN	14	-15.235	0.043	-21.735	1.00	0.31
ATOM	137	CG	ASN	14	-14.539	-0.346	-23.729	1.00	0.37
ATOM	138	OD1	ASN	14	-13.677	-0.981	-24.304	1.00	1.16
ATOM	139	ND2	ASN	14	-15.664	-0.077	-24.334	1.00	1.05
ATOM	140	HD21	ASN	14	-16.359	0.435	-23.871	1.00	1.81
ATOM	141	HD22	ASN	14	-15.812	-0.386	-25.252	1.00	1.06
ATOM	142	C	ASN	14	-12.813	-0.024	-20.309	1.00	0.22
ATOM	143	O	ASN	14	-13.566	-0.019	-19.357	1.00	0.23
ATOM	144	N	LEU	15	-11.630	0.533	-20.247	1.00	0.21
ATOM	145	HN	LEU	15	-11.042	0.517	-21.031	1.00	0.24
ATOM	146	CA	LEU	15	-11.171	1.194	-18.987	1.00	0.18
ATOM	147	HA	LEU	15	-12.025	1.447	-18.379	1.00	0.19
ATOM	148	CB	LEU	15	-10.250	0.243	-18.210	1.00	0.18
ATOM	149	HB1	LEU	15	-9.812	0.769	-17.375	1.00	0.19
ATOM	150	HB2	LEU	15	-9.463	-0.102	-18.865	1.00	0.21
ATOM	151	CG	LEU	15	-11.046	-0.964	-17.696	1.00	0.19
ATOM	152	HG	LEU	15	-11.547	-1.442	-18.525	1.00	0.20
ATOM	153	CD1	LEU	15	-10.086	-1.961	-17.044	1.00	0.20
ATOM	154	HD11	LEU	15	-9.726	-1.556	-16.110	1.00	0.98
ATOM	155	HD12	LEU	15	-9.251	-2.141	-17.704	1.00	1.04
ATOM	156	HD13	LEU	15	-10.604	-2.890	-16.857	1.00	1.07
ATOM	157	CD2	LEU	15	-12.083	-0.513	-16.658	1.00	0.21
ATOM	158	HD21	LEU	15	-12.114	-1.228	-15.850	1.00	1.07
ATOM	159	HD22	LEU	15	-13.055	-0.456	-17.122	1.00	1.00
ATOM	160	HD23	LEU	15	-11.814	0.457	-16.268	1.00	1.04
ATOM	161	C	LEU	15	-10.397	2.471	-19.334	1.00	0.18
ATOM	162	O	LEU	15	-9.785	2.570	-20.380	1.00	0.20
ATOM	163	N	THR	16	-10.425	3.447	-18.460	1.00	0.18
ATOM	164	HN	THR	16	-10.929	3.338	-17.627	1.00	0.18
ATOM	165	CA	THR	16	-9.699	4.729	-18.722	1.00	0.19
ATOM	166	HA	THR	16	-9.051	4.617	-19.574	1.00	0.20
ATOM	167	CB	THR	16	-10.716	5.839	-18.996	1.00	0.22
ATOM	168	HB	THR	16	-10.198	6.729	-19.315	1.00	0.24
ATOM	169	OG1	THR	16	-11.445	6.112	-17.808	1.00	0.23
ATOM	170	HG1	THR	16	-11.821	5.286	-17.495	1.00	0.98
ATOM	171	CG2	THR	16	-11.680	5.393	-20.096	1.00	0.26
ATOM	172	HG21	THR	16	-12.200	6.254	-20.489	1.00	1.05
ATOM	173	HG22	THR	16	-12.396	4.696	-19.686	1.00	1.02
ATOM	174	HG23	THR	16	-11.125	4.914	-20.889	1.00	1.05
ATOM	175	C	THR	16	-8.864	5.100	-17.495	1.00	0.17
ATOM	176	O	THR	16	-9.157	4.687	-16.391	1.00	0.16
ATOM	177	N	TYR	17	-7.826	5.878	-17.675	1.00	0.18
ATOM	178	HN	TYR	17	-7.603	6.202	-18.574	1.00	0.19
ATOM	179	CA	TYR	17	-6.981	6.268	-16.507	1.00	0.17
ATOM	180	HA	TYR	17	-7.585	6.233	-15.615	1.00	0.17
ATOM	181	CB	TYR	17	-5.814	5.288	-16.362	1.00	0.19
ATOM	182	HB1	TYR	17	-6.194	4.278	-16.347	1.00	0.19
ATOM	183	HB2	TYR	17	-5.292	5.488	-15.438	1.00	0.20
ATOM	184	CG	TYR	17	-4.857	5.445	-17.520	1.00	0.22
ATOM	185	CD1	TYR	17	-5.037	4.685	-18.682	1.00	0.26
ATOM	186	HD1	TYR	17	-5.867	3.998	-18.755	1.00	0.27
ATOM	187	CD2	TYR	17	-3.782	6.336	-17.426	1.00	0.25
ATOM	188	HD2	TYR	17	-3.643	6.923	-16.530	1.00	0.26
ATOM	189	CE1	TYR	17	-4.143	4.817	-19.751	1.00	0.31
ATOM	190	HE1	TYR	17	-4.282	4.231	-20.647	1.00	0.36
ATOM	191	CE2	TYR	17	-2.888	6.470	-18.496	1.00	0.30
ATOM	192	HE2	TYR	17	-2.059	7.158	-18.424	1.00	0.35
ATOM	193	CZ	TYR	17	-3.068	5.710	-19.658	1.00	0.32

ATOM	194	OH	TYR	17	-2.186	5.839	-20.711	1.00	0.39
ATOM	195	HH	TYR	17	-1.696	5.016	-20.790	1.00	0.85
ATOM	196	C	TYR	17	-6.448	7.692	-16.690	1.00	0.19
ATOM	197	O	TYR	17	-6.414	8.220	-17.784	1.00	0.21
ATOM	198	N	ARG	18	-6.044	8.320	-15.616	1.00	0.19
ATOM	199	HN	ARG	18	-6.089	7.874	-14.747	1.00	0.19
ATOM	200	CA	ARG	18	-5.523	9.714	-15.712	1.00	0.22
ATOM	201	HA	ARG	18	-5.131	9.877	-16.704	1.00	0.24
ATOM	202	CB	ARG	18	-6.674	10.691	-15.447	1.00	0.27
ATOM	203	HB1	ARG	18	-6.978	10.613	-14.412	1.00	0.31
ATOM	204	HB2	ARG	18	-7.507	10.442	-16.083	1.00	0.30
ATOM	205	CG	ARG	18	-6.229	12.127	-15.733	1.00	0.35
ATOM	206	HG1	ARG	18	-5.504	12.137	-16.531	1.00	0.93
ATOM	207	HG2	ARG	18	-5.790	12.549	-14.843	1.00	0.85
ATOM	208	CD	ARG	18	-7.447	12.946	-16.149	1.00	0.81
ATOM	209	HD1	ARG	18	-8.216	12.867	-15.378	1.00	1.29
ATOM	210	HD2	ARG	18	-7.838	12.561	-17.068	1.00	1.63
ATOM	211	NE	ARG	18	-7.030	14.362	-16.406	1.00	1.52
ATOM	212	HE	ARG	18	-7.071	14.711	-17.318	1.00	2.11
ATOM	213	CZ	ARG	18	-6.561	15.119	-15.456	1.00	2.24
ATOM	214	NH1	ARG	18	-6.119	16.314	-15.736	1.00	3.18
ATOM	215	HH11	ARG	18	-6.142	16.647	-16.679	1.00	3.48
ATOM	216	HH12	ARG	18	-5.760	16.898	-15.009	1.00	3.84
ATOM	217	NH2	ARG	18	-6.564	14.700	-14.220	1.00	2.63
ATOM	218	HH21	ARG	18	-6.928	13.795	-14.000	1.00	2.44
ATOM	219	HH22	ARG	18	-6.205	15.285	-13.493	1.00	3.49
ATOM	220	C	ARG	18	-4.413	9.931	-14.676	1.00	0.21
ATOM	221	O	ARG	18	-4.550	9.576	-13.522	1.00	0.23
ATOM	222	N	ILE	19	-3.314	10.514	-15.079	1.00	0.21
ATOM	223	HN	ILE	19	-3.223	10.794	-16.014	1.00	0.22
ATOM	224	CA	ILE	19	-2.196	10.755	-14.118	1.00	0.23
ATOM	225	HA	ILE	19	-2.200	9.985	-13.360	1.00	0.25
ATOM	226	CB	ILE	19	-0.864	10.721	-14.875	1.00	0.25
ATOM	227	HB	ILE	19	-0.862	11.491	-15.633	1.00	0.25
ATOM	228	CG1	ILE	19	-0.702	9.341	-15.531	1.00	0.29
ATOM	229	HG11	ILE	19	-1.607	9.092	-16.065	1.00	0.82
ATOM	230	HG12	ILE	19	-0.525	8.601	-14.765	1.00	0.97
ATOM	231	CG2	ILE	19	0.291	10.962	-13.893	1.00	0.29
ATOM	232	HG21	ILE	19	1.231	10.914	-14.420	1.00	1.08
ATOM	233	HG22	ILE	19	0.272	10.206	-13.123	1.00	1.09
ATOM	234	HG23	ILE	19	0.187	11.937	-13.440	1.00	1.00
ATOM	235	CD1	ILE	19	0.477	9.345	-16.512	1.00	0.93
ATOM	236	HD11	ILE	19	1.402	9.216	-15.970	1.00	1.59
ATOM	237	HD12	ILE	19	0.501	10.280	-17.050	1.00	1.50
ATOM	238	HD13	ILE	19	0.360	8.533	-17.214	1.00	1.55
ATOM	239	C	ILE	19	-2.381	12.126	-13.454	1.00	0.23
ATOM	240	O	ILE	19	-2.355	13.150	-14.108	1.00	0.23
ATOM	241	N	VAL	20	-2.563	12.152	-12.161	1.00	0.25
ATOM	242	HN	VAL	20	-2.578	11.314	-11.653	1.00	0.27
ATOM	243	CA	VAL	20	-2.746	13.454	-11.454	1.00	0.27
ATOM	244	HA	VAL	20	-3.496	14.035	-11.970	1.00	0.27
ATOM	245	CB	VAL	20	-3.202	13.205	-10.015	1.00	0.31
ATOM	246	HB	VAL	20	-2.522	12.517	-9.534	1.00	0.32
ATOM	247	CG1	VAL	20	-3.216	14.529	-9.247	1.00	0.33
ATOM	248	HG11	VAL	20	-3.607	15.310	-9.883	1.00	0.97
ATOM	249	HG12	VAL	20	-2.211	14.782	-8.944	1.00	1.08
ATOM	250	HG13	VAL	20	-3.842	14.432	-8.372	1.00	1.10
ATOM	251	CG2	VAL	20	-4.612	12.611	-10.028	1.00	0.33
ATOM	252	HG21	VAL	20	-5.296	13.317	-10.476	1.00	1.05
ATOM	253	HG22	VAL	20	-4.924	12.401	-9.016	1.00	1.03
ATOM	254	HG23	VAL	20	-4.612	11.697	-10.602	1.00	1.11
ATOM	255	C	VAL	20	-1.424	14.231	-11.451	1.00	0.27
ATOM	256	O	VAL	20	-1.403	15.435	-11.611	1.00	0.26
ATOM	257	N	ASN	21	-0.321	13.555	-11.259	1.00	0.28
ATOM	258	HN	ASN	21	-0.357	12.585	-11.124	1.00	0.30
ATOM	259	CA	ASN	21	0.992	14.265	-11.235	1.00	0.29
ATOM	260	HA	ASN	21	0.973	15.076	-11.949	1.00	0.26
ATOM	261	CB	ASN	21	1.235	14.829	-9.834	1.00	0.33
ATOM	262	HB1	ASN	21	0.544	15.637	-9.646	1.00	0.33
ATOM	263	HB2	ASN	21	2.249	15.199	-9.766	1.00	0.35
ATOM	264	CG	ASN	21	1.022	13.727	-8.795	1.00	0.40
ATOM	265	OD1	ASN	21	0.459	12.694	-9.097	1.00	1.01
ATOM	266	ND2	ASN	21	1.445	13.908	-7.574	1.00	0.88
ATOM	267	HD21	ASN	21	1.895	14.743	-7.330	1.00	1.50
ATOM	268	HD22	ASN	21	1.312	13.208	-6.901	1.00	0.88
ATOM	269	C	ASN	21	2.116	13.291	-11.606	1.00	0.34
ATOM	270	O	ASN	21	1.929	12.090	-11.619	1.00	0.37

ATOM	271	N	TYR	22	3.274	13.810	-11.933	1.00	0.38
ATOM	272	HN	TYR	22	3.387	14.783	-11.932	1.00	0.38
ATOM	273	CA	TYR	22	4.417	12.935	-12.340	1.00	0.46
ATOM	274	HA	TYR	22	4.067	11.929	-12.509	1.00	0.45
ATOM	275	CB	TYR	22	5.028	13.481	-13.630	1.00	0.49
ATOM	276	HB1	TYR	22	5.845	12.846	-13.938	1.00	0.56
ATOM	277	HB2	TYR	22	5.397	14.482	-13.457	1.00	0.53
ATOM	278	CG	TYR	22	3.981	13.513	-14.714	1.00	0.43
ATOM	279	CD1	TYR	22	3.684	12.352	-15.436	1.00	0.38
ATOM	280	HD1	TYR	22	4.199	11.430	-15.212	1.00	0.39
ATOM	281	CD2	TYR	22	3.313	14.708	-15.003	1.00	0.46
ATOM	282	HD2	TYR	22	3.543	15.603	-14.445	1.00	0.51
ATOM	283	CE1	TYR	22	2.718	12.386	-16.447	1.00	0.36
ATOM	284	HE1	TYR	22	2.490	11.491	-17.004	1.00	0.36
ATOM	285	CE2	TYR	22	2.345	14.742	-16.013	1.00	0.44
ATOM	286	HE2	TYR	22	1.828	15.663	-16.235	1.00	0.49
ATOM	287	CZ	TYR	22	2.048	13.581	-16.735	1.00	0.39
ATOM	288	OH	TYR	22	1.095	13.615	-17.733	1.00	0.43
ATOM	289	HH	TYR	22	1.173	14.457	-18.187	1.00	0.92
ATOM	290	C	TYR	22	5.499	12.923	-11.258	1.00	0.56
ATOM	291	O	TYR	22	6.554	12.378	-11.470	1.00	1.38
ATOM	292	N	THR	23	5.240	13.544	-10.130	1.00	0.47
ATOM	293	HN	THR	23	4.372	13.987	-10.023	1.00	1.08
ATOM	294	CA	THR	23	6.237	13.623	-9.004	1.00	0.46
ATOM	295	HA	THR	23	5.848	14.338	-8.304	1.00	0.48
ATOM	296	CB	THR	23	6.361	12.265	-8.273	1.00	0.62
ATOM	297	HB	THR	23	5.383	11.969	-7.921	1.00	0.68
ATOM	298	OG1	THR	23	7.223	12.420	-7.156	1.00	0.86
ATOM	299	HG1	THR	23	7.941	11.788	-7.244	1.00	1.28
ATOM	300	CG2	THR	23	6.916	11.159	-9.181	1.00	0.59
ATOM	301	HG21	THR	23	7.753	11.533	-9.748	1.00	1.08
ATOM	302	HG22	THR	23	6.141	10.816	-9.850	1.00	1.16
ATOM	303	HG23	THR	23	7.245	10.332	-8.570	1.00	1.22
ATOM	304	C	THR	23	7.623	14.115	-9.523	1.00	0.40
ATOM	305	O	THR	23	8.077	13.699	-10.565	1.00	0.45
ATOM	306	N	PRO	24	8.302	15.016	-8.823	1.00	0.42
ATOM	307	CA	PRO	24	9.625	15.520	-9.311	1.00	0.42
ATOM	308	HA	PRO	24	9.534	15.918	-10.307	1.00	0.46
ATOM	309	CB	PRO	24	9.924	16.655	-8.335	1.00	0.50
ATOM	310	HB1	PRO	24	9.743	17.605	-8.815	1.00	0.57
ATOM	311	HB2	PRO	24	10.955	16.598	-8.014	1.00	0.49
ATOM	312	CG	PRO	24	8.995	16.507	-7.129	1.00	0.66
ATOM	313	HG1	PRO	24	8.613	17.475	-6.842	1.00	0.84
ATOM	314	HG2	PRO	24	9.537	16.069	-6.303	1.00	0.76
ATOM	315	CD	PRO	24	7.832	15.598	-7.529	1.00	0.56
ATOM	316	HD2	PRO	24	7.675	14.826	-6.786	1.00	0.62
ATOM	317	HD1	PRO	24	6.940	16.183	-7.680	1.00	0.61
ATOM	318	C	PRO	24	10.743	14.470	-9.253	1.00	0.40
ATOM	319	O	PRO	24	11.835	14.692	-9.737	1.00	0.40
ATOM	320	N	ASP	25	10.490	13.337	-8.662	1.00	0.44
ATOM	321	HN	ASP	25	9.608	13.172	-8.270	1.00	0.48
ATOM	322	CA	ASP	25	11.554	12.295	-8.577	1.00	0.48
ATOM	323	HA	ASP	25	12.393	12.695	-8.025	1.00	0.51
ATOM	324	CB	ASP	25	11.016	11.062	-7.847	1.00	0.57
ATOM	325	HB1	ASP	25	11.719	10.249	-7.945	1.00	0.61
ATOM	326	HB2	ASP	25	10.068	10.773	-8.276	1.00	0.56
ATOM	327	CG	ASP	25	10.827	11.394	-6.364	1.00	0.67
ATOM	328	OD1	ASP	25	10.079	10.689	-5.709	1.00	1.23
ATOM	329	OD2	ASP	25	11.437	12.348	-5.908	1.00	1.34
ATOM	330	C	ASP	25	12.025	11.916	-9.985	1.00	0.45
ATOM	331	O	ASP	25	13.179	11.597	-10.191	1.00	0.55
ATOM	332	N	MET	26	11.146	11.948	-10.955	1.00	0.40
ATOM	333	HN	MET	26	10.220	12.209	-10.767	1.00	0.41
ATOM	334	CA	MET	26	11.553	11.590	-12.348	1.00	0.42
ATOM	335	HA	MET	26	12.624	11.686	-12.447	1.00	0.49
ATOM	336	CB	MET	26	11.144	10.149	-12.656	1.00	0.53
ATOM	337	HB1	MET	26	11.282	9.954	-13.709	1.00	0.55
ATOM	338	HB2	MET	26	10.105	10.006	-12.397	1.00	0.51
ATOM	339	CG	MET	26	12.011	9.186	-11.846	1.00	0.71
ATOM	340	HG1	MET	26	11.783	9.288	-10.796	1.00	0.73
ATOM	341	HG2	MET	26	13.053	9.419	-12.009	1.00	0.77
ATOM	342	SD	MET	26	11.683	7.485	-12.380	1.00	0.89
ATOM	343	CE	MET	26	10.000	7.330	-11.728	1.00	0.59
ATOM	344	HE1	MET	26	9.292	7.456	-12.534	1.00	1.25
ATOM	345	HE2	MET	26	9.825	8.084	-10.979	1.00	1.23
ATOM	346	HE3	MET	26	9.877	6.352	-11.285	1.00	1.23
ATOM	347	C	MET	26	10.872	12.530	-13.344	1.00	0.34

ATOM	348	O	MET	26	9.897	13.184	-13.031	1.00	0.32
ATOM	349	N	THR	27	11.385	12.604	-14.544	1.00	0.33
ATOM	350	HN	THR	27	12.174	12.070	-14.773	1.00	0.38
ATOM	351	CA	THR	27	10.775	13.504	-15.562	1.00	0.32
ATOM	352	HA	THR	27	10.618	14.483	-15.133	1.00	0.35
ATOM	353	CB	THR	27	11.711	13.616	-16.768	1.00	0.39
ATOM	354	HB	THR	27	11.295	14.308	-17.484	1.00	0.42
ATOM	355	OG1	THR	27	11.852	12.338	-17.371	1.00	0.37
ATOM	356	HG1	THR	27	12.765	12.242	-17.653	1.00	0.94
ATOM	357	CG2	THR	27	13.080	14.121	-16.313	1.00	0.51
ATOM	358	HG21	THR	27	13.602	14.553	-17.154	1.00	1.14
ATOM	359	HG22	THR	27	13.655	13.297	-15.918	1.00	1.11
ATOM	360	HG23	THR	27	12.951	14.871	-15.546	1.00	1.12
ATOM	361	C	THR	27	9.436	12.921	-16.013	1.00	0.27
ATOM	362	O	THR	27	9.177	11.743	-15.864	1.00	0.24
ATOM	363	N	HIS	28	8.580	13.740	-16.554	1.00	0.32
ATOM	364	HN	HIS	28	8.807	14.688	-16.657	1.00	0.37
ATOM	365	CA	HIS	28	7.253	13.241	-17.004	1.00	0.34
ATOM	366	HA	HIS	28	6.715	12.833	-16.161	1.00	0.36
ATOM	367	CB	HIS	28	6.457	14.403	-17.601	1.00	0.46
ATOM	368	HB1	HIS	28	5.428	14.104	-17.736	1.00	0.71
ATOM	369	HB2	HIS	28	6.880	14.676	-18.557	1.00	0.88
ATOM	370	CG	HIS	28	6.516	15.583	-16.669	1.00	0.73
ATOM	371	ND1	HIS	28	6.056	16.838	-17.036	1.00	1.66
ATOM	372	HD1	HIS	28	5.659	17.080	-17.898	1.00	2.30
ATOM	373	CD2	HIS	28	6.987	15.716	-15.387	1.00	1.33
ATOM	374	HD2	HIS	28	7.423	14.922	-14.798	1.00	2.01
ATOM	375	CE1	HIS	28	6.258	17.664	-15.993	1.00	1.95
ATOM	376	HE1	HIS	28	5.993	18.711	-15.990	1.00	2.70
ATOM	377	NE2	HIS	28	6.823	17.031	-14.962	1.00	1.71
ATOM	378	C	HIS	28	7.436	12.156	-18.069	1.00	0.30
ATOM	379	O	HIS	28	6.737	11.164	-18.082	1.00	0.30
ATOM	380	N	SER	29	8.362	12.338	-18.970	1.00	0.31
ATOM	381	HN	SER	29	8.912	13.149	-18.952	1.00	0.34
ATOM	382	CA	SER	29	8.567	11.319	-20.039	1.00	0.32
ATOM	383	HA	SER	29	7.660	11.217	-20.615	1.00	0.35
ATOM	384	CB	SER	29	9.699	11.775	-20.959	1.00	0.38
ATOM	385	HB1	SER	29	9.973	10.963	-21.621	1.00	0.39
ATOM	386	HB2	SER	29	10.555	12.056	-20.368	1.00	0.37
ATOM	387	OG	SER	29	9.265	12.896	-21.717	1.00	0.45
ATOM	388	HG	SER	29	9.157	12.614	-22.628	1.00	0.96
ATOM	389	C	SER	29	8.931	9.964	-19.424	1.00	0.26
ATOM	390	O	SER	29	8.479	8.930	-19.876	1.00	0.26
ATOM	391	N	GLU	30	9.747	9.954	-18.405	1.00	0.24
ATOM	392	HN	GLU	30	10.107	10.796	-18.056	1.00	0.25
ATOM	393	CA	GLU	30	10.137	8.657	-17.779	1.00	0.22
ATOM	394	HA	GLU	30	10.484	7.978	-18.542	1.00	0.25
ATOM	395	CB	GLU	30	11.260	8.899	-16.769	1.00	0.23
ATOM	396	HB1	GLU	30	11.424	8.002	-16.191	1.00	0.24
ATOM	397	HB2	GLU	30	10.980	9.707	-16.108	1.00	0.22
ATOM	398	CG	GLU	30	12.547	9.268	-17.510	1.00	0.29
ATOM	399	HG1	GLU	30	12.386	10.165	-18.086	1.00	0.67
ATOM	400	HG2	GLU	30	12.826	8.460	-18.171	1.00	0.68
ATOM	401	CD	GLU	30	13.666	9.509	-16.495	1.00	0.84
ATOM	402	OE1	GLU	30	13.436	9.266	-15.321	1.00	1.49
ATOM	403	OE2	GLU	30	14.731	9.936	-16.908	1.00	1.59
ATOM	404	C	GLU	30	8.935	8.046	-17.051	1.00	0.17
ATOM	405	O	GLU	30	8.715	6.849	-17.082	1.00	0.19
ATOM	406	N	VAL	31	8.163	8.861	-16.387	1.00	0.16
ATOM	407	HN	VAL	31	8.366	9.819	-16.371	1.00	0.17
ATOM	408	CA	VAL	31	6.983	8.341	-15.640	1.00	0.16
ATOM	409	HA	VAL	31	7.292	7.527	-14.999	1.00	0.17
ATOM	410	CB	VAL	31	6.402	9.464	-14.782	1.00	0.20
ATOM	411	HB	VAL	31	6.261	10.344	-15.392	1.00	0.22
ATOM	412	CG1	VAL	31	5.058	9.021	-14.208	1.00	0.23
ATOM	413	HG11	VAL	31	5.135	8.000	-13.867	1.00	0.97
ATOM	414	HG12	VAL	31	4.298	9.090	-14.973	1.00	1.07
ATOM	415	HG13	VAL	31	4.793	9.659	-13.378	1.00	1.07
ATOM	416	CG2	VAL	31	7.364	9.785	-13.636	1.00	0.24
ATOM	417	HG21	VAL	31	7.528	8.897	-13.045	1.00	1.05
ATOM	418	HG22	VAL	31	6.936	10.557	-13.013	1.00	1.03
ATOM	419	HG23	VAL	31	8.304	10.129	-14.040	1.00	0.99
ATOM	420	C	VAL	31	5.911	7.844	-16.617	1.00	0.16
ATOM	421	O	VAL	31	5.293	6.817	-16.406	1.00	0.17
ATOM	422	N	GLU	32	5.672	8.571	-17.677	1.00	0.18
ATOM	423	HN	GLU	32	6.172	9.401	-17.824	1.00	0.19
ATOM	424	CA	GLU	32	4.626	8.146	-18.652	1.00	0.21

ATOM	425	HA	GLU	32	3.673	8.092	-18.147	1.00	0.24
ATOM	426	CB	GLU	32	4.533	9.170	-19.787	1.00	0.27
ATOM	427	HB1	GLU	32	3.922	8.772	-20.582	1.00	0.31
ATOM	428	HB2	GLU	32	5.524	9.379	-20.164	1.00	0.28
ATOM	429	CG	GLU	32	3.904	10.463	-19.262	1.00	0.29
ATOM	430	HG1	GLU	32	4.456	10.812	-18.405	1.00	0.48
ATOM	431	HG2	GLU	32	2.879	10.272	-18.977	1.00	0.52
ATOM	432	CD	GLU	32	3.937	11.529	-20.359	1.00	0.70
ATOM	433	OE1	GLU	32	4.969	12.161	-20.513	1.00	1.37
ATOM	434	OE2	GLU	32	2.929	11.696	-21.026	1.00	1.45
ATOM	435	C	GLU	32	4.962	6.773	-19.235	1.00	0.20
ATOM	436	O	GLU	32	4.126	5.893	-19.280	1.00	0.20
ATOM	437	N	LYS	33	6.168	6.575	-19.689	1.00	0.20
ATOM	438	HN	LYS	33	6.835	7.293	-19.654	1.00	0.21
ATOM	439	CA	LYS	33	6.518	5.249	-20.269	1.00	0.21
ATOM	440	HA	LYS	33	5.825	5.029	-21.068	1.00	0.24
ATOM	441	CB	LYS	33	7.940	5.281	-20.843	1.00	0.26
ATOM	442	HB1	LYS	33	7.987	6.024	-21.624	1.00	0.31
ATOM	443	HB2	LYS	33	8.179	4.312	-21.257	1.00	0.31
ATOM	444	CG	LYS	33	8.954	5.631	-19.748	1.00	0.26
ATOM	445	HG1	LYS	33	8.823	4.970	-18.906	1.00	0.40
ATOM	446	HG2	LYS	33	8.799	6.648	-19.430	1.00	0.42
ATOM	447	CD	LYS	33	10.380	5.469	-20.291	1.00	0.48
ATOM	448	HD1	LYS	33	10.466	4.517	-20.793	1.00	0.74
ATOM	449	HD2	LYS	33	11.080	5.505	-19.469	1.00	1.11
ATOM	450	CE	LYS	33	10.705	6.593	-21.282	1.00	0.92
ATOM	451	HE1	LYS	33	10.398	7.543	-20.868	1.00	1.52
ATOM	452	HE2	LYS	33	10.184	6.419	-22.211	1.00	1.19
ATOM	453	NZ	LYS	33	12.172	6.614	-21.538	1.00	1.60
ATOM	454	HZ1	LYS	33	12.668	6.957	-20.692	1.00	1.99
ATOM	455	HZ2	LYS	33	12.374	7.247	-22.340	1.00	2.14
ATOM	456	HZ3	LYS	33	12.498	5.653	-21.763	1.00	2.03
ATOM	457	C	LYS	33	6.399	4.158	-19.202	1.00	0.19
ATOM	458	O	LYS	33	6.054	3.035	-19.495	1.00	0.20
ATOM	459	N	ALA	34	6.682	4.471	-17.966	1.00	0.17
ATOM	460	HN	ALA	34	6.965	5.383	-17.740	1.00	0.18
ATOM	461	CA	ALA	34	6.589	3.428	-16.904	1.00	0.16
ATOM	462	HA	ALA	34	7.276	2.625	-17.128	1.00	0.18
ATOM	463	CB	ALA	34	6.952	4.043	-15.551	1.00	0.16
ATOM	464	HB1	ALA	34	6.483	3.476	-14.761	1.00	1.02
ATOM	465	HB2	ALA	34	6.604	5.065	-15.516	1.00	0.98
ATOM	466	HB3	ALA	34	8.024	4.022	-15.423	1.00	1.02
ATOM	467	C	ALA	34	5.164	2.875	-16.844	1.00	0.16
ATOM	468	O	ALA	34	4.954	1.677	-16.847	1.00	0.17
ATOM	469	N	PHE	35	4.182	3.729	-16.792	1.00	0.16
ATOM	470	HN	PHE	35	4.364	4.694	-16.792	1.00	0.16
ATOM	471	CA	PHE	35	2.781	3.230	-16.736	1.00	0.17
ATOM	472	HA	PHE	35	2.690	2.525	-15.924	1.00	0.17
ATOM	473	CB	PHE	35	1.815	4.396	-16.508	1.00	0.18
ATOM	474	HB1	PHE	35	0.802	4.060	-16.672	1.00	0.19
ATOM	475	HB2	PHE	35	2.045	5.192	-17.200	1.00	0.19
ATOM	476	CG	PHE	35	1.953	4.902	-15.089	1.00	0.18
ATOM	477	CD1	PHE	35	1.616	4.071	-14.011	1.00	0.19
ATOM	478	HD1	PHE	35	1.258	3.069	-14.191	1.00	0.19
ATOM	479	CD2	PHE	35	2.415	6.203	-14.849	1.00	0.20
ATOM	480	HD2	PHE	35	2.674	6.847	-15.677	1.00	0.21
ATOM	481	CE1	PHE	35	1.743	4.539	-12.699	1.00	0.21
ATOM	482	HE1	PHE	35	1.484	3.897	-11.870	1.00	0.23
ATOM	483	CE2	PHE	35	2.540	6.670	-13.535	1.00	0.22
ATOM	484	HE2	PHE	35	2.893	7.672	-13.349	1.00	0.24
ATOM	485	CZ	PHE	35	2.205	5.838	-12.460	1.00	0.22
ATOM	486	HZ	PHE	35	2.303	6.198	-11.447	1.00	0.24
ATOM	487	C	PHE	35	2.432	2.524	-18.048	1.00	0.18
ATOM	488	O	PHE	35	1.770	1.507	-18.055	1.00	0.19
ATOM	489	N	LYS	36	2.864	3.053	-19.162	1.00	0.19
ATOM	490	HN	LYS	36	3.394	3.878	-19.144	1.00	0.19
ATOM	491	CA	LYS	36	2.535	2.399	-20.460	1.00	0.22
ATOM	492	HA	LYS	36	1.462	2.358	-20.574	1.00	0.23
ATOM	493	CB	LYS	36	3.135	3.205	-21.614	1.00	0.24
ATOM	494	HB1	LYS	36	3.045	2.641	-22.530	1.00	0.27
ATOM	495	HB2	LYS	36	4.178	3.400	-21.412	1.00	0.24
ATOM	496	CG	LYS	36	2.384	4.530	-21.758	1.00	0.27
ATOM	497	HG1	LYS	36	2.471	5.097	-20.844	1.00	0.69
ATOM	498	HG2	LYS	36	1.341	4.332	-21.963	1.00	0.68
ATOM	499	CD	LYS	36	2.988	5.332	-22.913	1.00	0.75
ATOM	500	HD1	LYS	36	2.898	4.766	-23.828	1.00	1.39
ATOM	501	HD2	LYS	36	4.032	5.525	-22.710	1.00	1.34

ATOM	502	CE	LYS	36	2.243	6.659	-23.065	1.00	1.15
ATOM	503	HE1	LYS	36	2.728	7.415	-22.464	1.00	1.64
ATOM	504	HE2	LYS	36	1.221	6.540	-22.736	1.00	1.61
ATOM	505	NZ	LYS	36	2.260	7.076	-24.496	1.00	1.99
ATOM	506	HZ1	LYS	36	2.628	6.298	-25.079	1.00	2.51
ATOM	507	HZ2	LYS	36	2.871	7.911	-24.605	1.00	2.40
ATOM	508	HZ3	LYS	36	1.295	7.309	-24.801	1.00	2.38
ATOM	509	C	LYS	36	3.098	0.976	-20.481	1.00	0.21
ATOM	510	O	LYS	36	2.446	0.053	-20.927	1.00	0.23
ATOM	511	N	LYS	37	4.295	0.778	-19.995	1.00	0.21
ATOM	512	HN	LYS	37	4.810	1.527	-19.629	1.00	0.20
ATOM	513	CA	LYS	37	4.864	-0.600	-19.988	1.00	0.22
ATOM	514	HA	LYS	37	4.926	-0.974	-21.000	1.00	0.24
ATOM	515	CB	LYS	37	6.257	-0.581	-19.358	1.00	0.22
ATOM	516	HB1	LYS	37	6.589	-1.596	-19.195	1.00	0.24
ATOM	517	HB2	LYS	37	6.216	-0.061	-18.412	1.00	0.21
ATOM	518	CG	LYS	37	7.244	0.130	-20.285	1.00	0.26
ATOM	519	HG1	LYS	37	6.921	1.140	-20.459	1.00	0.25
ATOM	520	HG2	LYS	37	7.296	-0.398	-21.227	1.00	0.28
ATOM	521	CD	LYS	37	8.625	0.139	-19.628	1.00	0.30
ATOM	522	HD1	LYS	37	8.994	-0.873	-19.551	1.00	0.77
ATOM	523	HD2	LYS	37	8.549	0.570	-18.640	1.00	0.84
ATOM	524	CE	LYS	37	9.594	0.968	-20.473	1.00	0.90
ATOM	525	HE1	LYS	37	10.530	1.076	-19.943	1.00	1.47
ATOM	526	HE2	LYS	37	9.169	1.945	-20.652	1.00	1.59
ATOM	527	NZ	LYS	37	9.836	0.286	-21.774	1.00	1.77
ATOM	528	HZ1	LYS	37	9.798	0.984	-22.543	1.00	2.22
ATOM	529	HZ2	LYS	37	9.106	-0.439	-21.926	1.00	2.28
ATOM	530	HZ3	LYS	37	10.774	-0.161	-21.762	1.00	2.33
ATOM	531	C	LYS	37	3.955	-1.506	-19.158	1.00	0.20
ATOM	532	O	LYS	37	3.689	-2.636	-19.516	1.00	0.21
ATOM	533	N	ALA	38	3.479	-1.013	-18.046	1.00	0.19
ATOM	534	HN	ALA	38	3.711	-0.098	-17.777	1.00	0.19
ATOM	535	CA	ALA	38	2.589	-1.838	-17.182	1.00	0.18
ATOM	536	HA	ALA	38	3.116	-2.727	-16.870	1.00	0.19
ATOM	537	CB	ALA	38	2.183	-1.030	-15.949	1.00	0.19
ATOM	538	HB1	ALA	38	2.831	-0.172	-15.851	1.00	1.05
ATOM	539	HB2	ALA	38	2.270	-1.649	-15.068	1.00	1.00
ATOM	540	HB3	ALA	38	1.161	-0.698	-16.057	1.00	1.06
ATOM	541	C	ALA	38	1.338	-2.238	-17.965	1.00	0.18
ATOM	542	O	ALA	38	0.967	-3.392	-18.012	1.00	0.19
ATOM	543	N	PHE	39	0.688	-1.295	-18.589	1.00	0.18
ATOM	544	HN	PHE	39	1.005	-0.368	-18.547	1.00	0.18
ATOM	545	CA	PHE	39	-0.535	-1.632	-19.367	1.00	0.19
ATOM	546	HA	PHE	39	-1.248	-2.122	-18.720	1.00	0.19
ATOM	547	CB	PHE	39	-1.156	-0.354	-19.937	1.00	0.21
ATOM	548	HB1	PHE	39	-1.883	-0.614	-20.692	1.00	0.24
ATOM	549	HB2	PHE	39	-0.381	0.256	-20.378	1.00	0.21
ATOM	550	CG	PHE	39	-1.836	0.416	-18.829	1.00	0.20
ATOM	551	CD1	PHE	39	-3.010	-0.080	-18.250	1.00	0.25
ATOM	552	HD1	PHE	39	-3.429	-1.014	-18.595	1.00	0.30
ATOM	553	CD2	PHE	39	-1.294	1.627	-18.380	1.00	0.17
ATOM	554	HD2	PHE	39	-0.389	2.012	-18.827	1.00	0.18
ATOM	555	CE1	PHE	39	-3.642	0.633	-17.224	1.00	0.28
ATOM	556	HE1	PHE	39	-4.548	0.250	-16.779	1.00	0.34
ATOM	557	CE2	PHE	39	-1.926	2.341	-17.354	1.00	0.18
ATOM	558	HE2	PHE	39	-1.507	3.275	-17.007	1.00	0.17
ATOM	559	CZ	PHE	39	-3.099	1.843	-16.776	1.00	0.23
ATOM	560	HZ	PHE	39	-3.587	2.394	-15.985	1.00	0.26
ATOM	561	C	PHE	39	-0.154	-2.571	-20.508	1.00	0.18
ATOM	562	O	PHE	39	-0.862	-3.509	-20.817	1.00	0.18
ATOM	563	N	LYS	40	0.963	-2.330	-21.136	1.00	0.19
ATOM	564	HN	LYS	40	1.522	-1.570	-20.870	1.00	0.19
ATOM	565	CA	LYS	40	1.388	-3.214	-22.254	1.00	0.19
ATOM	566	HA	LYS	40	0.642	-3.186	-23.031	1.00	0.20
ATOM	567	CB	LYS	40	2.730	-2.707	-22.804	1.00	0.21
ATOM	568	HB1	LYS	40	3.466	-2.723	-22.014	1.00	0.21
ATOM	569	HB2	LYS	40	2.610	-1.692	-23.155	1.00	0.25
ATOM	570	CG	LYS	40	3.218	-3.588	-23.966	1.00	0.25
ATOM	571	HG1	LYS	40	3.337	-4.604	-23.621	1.00	0.46
ATOM	572	HG2	LYS	40	4.171	-3.218	-24.314	1.00	0.46
ATOM	573	CD	LYS	40	2.213	-3.560	-25.121	1.00	0.38
ATOM	574	HD1	LYS	40	1.840	-2.555	-25.253	1.00	0.54
ATOM	575	HD2	LYS	40	1.392	-4.227	-24.905	1.00	0.56
ATOM	576	CE	LYS	40	2.903	-4.019	-26.407	1.00	0.40
ATOM	577	HE1	LYS	40	3.776	-4.604	-26.158	1.00	1.07
ATOM	578	HE2	LYS	40	3.199	-3.157	-26.885	1.00	1.03

ATOM	579	NZ	LYS	40	1.958	-4.852	-27.203	1.00	1.40
ATOM	580	HZ1	LYS	40	1.571	-5.607	-26.602	1.00	1.95
ATOM	581	HZ2	LYS	40	2.464	-5.274	-28.009	1.00	1.92
ATOM	582	HZ3	LYS	40	1.181	-4.258	-27.552	1.00	2.02
ATOM	583	C	LYS	40	1.553	-4.648	-21.740	1.00	0.17
ATOM	584	O	LYS	40	1.034	-5.583	-22.314	1.00	0.17
ATOM	585	N	VAL	41	2.271	-4.828	-20.663	1.00	0.17
ATOM	586	HN	VAL	41	2.681	-4.060	-20.214	1.00	0.18
ATOM	587	CA	VAL	41	2.468	-6.204	-20.116	1.00	0.16
ATOM	588	HA	VAL	41	2.953	-6.816	-20.862	1.00	0.17
ATOM	589	CB	VAL	41	3.350	-6.143	-18.868	1.00	0.18
ATOM	590	HB	VAL	41	2.966	-5.393	-18.192	1.00	0.41
ATOM	591	CG1	VAL	41	3.343	-7.508	-18.175	1.00	0.44
ATOM	592	HG11	VAL	41	2.420	-7.631	-17.629	1.00	1.16
ATOM	593	HG12	VAL	41	4.176	-7.571	-17.490	1.00	1.18
ATOM	594	HG13	VAL	41	3.429	-8.289	-18.916	1.00	1.11
ATOM	595	CG2	VAL	41	4.781	-5.785	-19.277	1.00	0.43
ATOM	596	HG21	VAL	41	5.132	-6.492	-20.013	1.00	1.12
ATOM	597	HG22	VAL	41	5.423	-5.820	-18.411	1.00	1.11
ATOM	598	HG23	VAL	41	4.797	-4.790	-19.697	1.00	1.19
ATOM	599	C	VAL	41	1.122	-6.833	-19.751	1.00	0.16
ATOM	600	O	VAL	41	0.887	-7.999	-19.996	1.00	0.17
ATOM	601	N	TRP	42	0.240	-6.080	-19.152	1.00	0.16
ATOM	602	HN	TRP	42	0.448	-5.143	-18.950	1.00	0.17
ATOM	603	CA	TRP	42	-1.079	-6.655	-18.761	1.00	0.17
ATOM	604	HA	TRP	42	-0.927	-7.642	-18.352	1.00	0.17
ATOM	605	CB	TRP	42	-1.739	-5.767	-17.699	1.00	0.18
ATOM	606	HB1	TRP	42	-2.787	-6.018	-17.621	1.00	0.19
ATOM	607	HB2	TRP	42	-1.638	-4.730	-17.983	1.00	0.20
ATOM	608	CG	TRP	42	-1.073	-5.990	-16.377	1.00	0.18
ATOM	609	CD1	TRP	42	-0.311	-5.082	-15.724	1.00	0.22
ATOM	610	HD1	TRP	42	-0.092	-4.084	-16.066	1.00	0.28
ATOM	611	CD2	TRP	42	-1.095	-7.182	-15.539	1.00	0.19
ATOM	612	NE1	TRP	42	0.140	-5.643	-14.543	1.00	0.22
ATOM	613	HE1	TRP	42	0.714	-5.194	-13.887	1.00	0.25
ATOM	614	CE2	TRP	42	-0.315	-6.935	-14.384	1.00	0.20
ATOM	615	CE3	TRP	42	-1.707	-8.441	-15.669	1.00	0.25
ATOM	616	HE3	TRP	42	-2.309	-8.658	-16.539	1.00	0.27
ATOM	617	CZ2	TRP	42	-0.149	-7.903	-13.393	1.00	0.24
ATOM	618	HZ2	TRP	42	0.454	-7.691	-12.521	1.00	0.25
ATOM	619	CZ3	TRP	42	-1.543	-9.418	-14.673	1.00	0.31
ATOM	620	HZ3	TRP	42	-2.018	-10.381	-14.782	1.00	0.39
ATOM	621	CH2	TRP	42	-0.764	-9.149	-13.538	1.00	0.30
ATOM	622	HH2	TRP	42	-0.642	-9.904	-12.775	1.00	0.35
ATOM	623	C	TRP	42	-1.991	-6.754	-19.985	1.00	0.17
ATOM	624	O	TRP	42	-2.726	-7.706	-20.138	1.00	0.18
ATOM	625	N	SER	43	-1.952	-5.782	-20.855	1.00	0.17
ATOM	626	HN	SER	43	-1.352	-5.021	-20.713	1.00	0.17
ATOM	627	CA	SER	43	-2.831	-5.825	-22.062	1.00	0.18
ATOM	628	HA	SER	43	-3.846	-6.028	-21.759	1.00	0.19
ATOM	629	CB	SER	43	-2.779	-4.474	-22.775	1.00	0.20
ATOM	630	HB1	SER	43	-2.965	-3.683	-22.059	1.00	0.21
ATOM	631	HB2	SER	43	-3.533	-4.442	-23.543	1.00	0.23
ATOM	632	OG	SER	43	-1.499	-4.304	-23.368	1.00	0.21
ATOM	633	HG	SER	43	-1.031	-5.140	-23.309	1.00	0.97
ATOM	634	C	SER	43	-2.358	-6.922	-23.019	1.00	0.18
ATOM	635	O	SER	43	-3.085	-7.350	-23.893	1.00	0.21
ATOM	636	N	ASP	44	-1.148	-7.379	-22.866	1.00	0.17
ATOM	637	HN	ASP	44	-0.575	-7.019	-22.156	1.00	0.18
ATOM	638	CA	ASP	44	-0.632	-8.445	-23.770	1.00	0.18
ATOM	639	HA	ASP	44	-0.650	-8.086	-24.788	1.00	0.19
ATOM	640	CB	ASP	44	0.809	-8.793	-23.386	1.00	0.20
ATOM	641	HB1	ASP	44	1.117	-9.683	-23.915	1.00	0.21
ATOM	642	HB2	ASP	44	0.864	-8.969	-22.322	1.00	0.22
ATOM	643	CG	ASP	44	1.734	-7.635	-23.760	1.00	0.24
ATOM	644	OD1	ASP	44	1.340	-6.833	-24.591	1.00	0.85
ATOM	645	OD2	ASP	44	2.820	-7.568	-23.209	1.00	0.84
ATOM	646	C	ASP	44	-1.499	-9.705	-23.665	1.00	0.19
ATOM	647	O	ASP	44	-1.753	-10.366	-24.653	1.00	0.21
ATOM	648	N	VAL	45	-1.927	-10.058	-22.475	1.00	0.21
ATOM	649	HN	VAL	45	-1.689	-9.519	-21.693	1.00	0.21
ATOM	650	CA	VAL	45	-2.749	-11.299	-22.302	1.00	0.26
ATOM	651	HA	VAL	45	-2.833	-11.811	-23.247	1.00	0.28
ATOM	652	CB	VAL	45	-2.045	-12.222	-21.303	1.00	0.30
ATOM	653	HB	VAL	45	-2.645	-13.107	-21.146	1.00	0.37
ATOM	654	CG1	VAL	45	-0.678	-12.626	-21.866	1.00	0.36
ATOM	655	HG11	VAL	45	-0.210	-11.766	-22.323	1.00	1.07

ATOM	656	HG12	VAL	45	-0.810	-13.400	-22.607	1.00	1.02
ATOM	657	HG13	VAL	45	-0.051	-12.995	-21.068	1.00	1.13
ATOM	658	CG2	VAL	45	-1.855	-11.486	-19.973	1.00	0.32
ATOM	659	HG21	VAL	45	-2.819	-11.303	-19.524	1.00	0.96
ATOM	660	HG22	VAL	45	-1.356	-10.545	-20.149	1.00	1.09
ATOM	661	HG23	VAL	45	-1.258	-12.091	-19.305	1.00	1.11
ATOM	662	C	VAL	45	-4.160	-10.966	-21.790	1.00	0.29
ATOM	663	O	VAL	45	-4.837	-11.819	-21.249	1.00	0.64
ATOM	664	N	THR	46	-4.619	-9.748	-21.963	1.00	0.36
ATOM	665	HN	THR	46	-4.062	-9.076	-22.409	1.00	0.65
ATOM	666	CA	THR	46	-5.998	-9.382	-21.491	1.00	0.38
ATOM	667	HA	THR	46	-6.567	-10.277	-21.320	1.00	0.44
ATOM	668	CB	THR	46	-5.912	-8.577	-20.186	1.00	0.39
ATOM	669	HB	THR	46	-6.889	-8.193	-19.943	1.00	0.46
ATOM	670	OG1	THR	46	-5.018	-7.491	-20.358	1.00	0.36
ATOM	671	HG1	THR	46	-5.532	-6.719	-20.608	1.00	0.94
ATOM	672	CG2	THR	46	-5.430	-9.461	-19.036	1.00	0.43
ATOM	673	HG21	THR	46	-4.929	-10.327	-19.429	1.00	1.08
ATOM	674	HG22	THR	46	-6.277	-9.775	-18.445	1.00	1.15
ATOM	675	HG23	THR	46	-4.746	-8.901	-18.415	1.00	1.05
ATOM	676	C	THR	46	-6.668	-8.482	-22.553	1.00	0.32
ATOM	677	O	THR	46	-6.124	-7.450	-22.892	1.00	0.32
ATOM	678	N	PRO	47	-7.833	-8.829	-23.084	1.00	0.30
ATOM	679	CA	PRO	47	-8.479	-7.951	-24.100	1.00	0.30
ATOM	680	HA	PRO	47	-7.820	-7.790	-24.936	1.00	0.33
ATOM	681	CB	PRO	47	-9.687	-8.773	-24.546	1.00	0.35
ATOM	682	HB1	PRO	47	-9.541	-9.110	-25.561	1.00	0.40
ATOM	683	HB2	PRO	47	-10.579	-8.166	-24.489	1.00	0.37
ATOM	684	CG	PRO	47	-9.825	-9.986	-23.621	1.00	0.35
ATOM	685	HG1	PRO	47	-9.916	-10.885	-24.212	1.00	0.42
ATOM	686	HG2	PRO	47	-10.703	-9.869	-23.001	1.00	0.34
ATOM	687	CD	PRO	47	-8.576	-10.077	-22.739	1.00	0.33
ATOM	688	HD2	PRO	47	-8.853	-10.091	-21.692	1.00	0.31
ATOM	689	HD1	PRO	47	-7.993	-10.946	-22.999	1.00	0.39
ATOM	690	C	PRO	47	-8.933	-6.614	-23.506	1.00	0.25
ATOM	691	O	PRO	47	-9.744	-5.914	-24.080	1.00	0.26
ATOM	692	N	LEU	48	-8.418	-6.252	-22.362	1.00	0.26
ATOM	693	HN	LEU	48	-7.766	-6.828	-21.912	1.00	0.29
ATOM	694	CA	LEU	48	-8.827	-4.960	-21.742	1.00	0.26
ATOM	695	HA	LEU	48	-9.904	-4.905	-21.696	1.00	0.27
ATOM	696	CB	LEU	48	-8.241	-4.858	-20.329	1.00	0.31
ATOM	697	HB1	LEU	48	-8.476	-3.892	-19.909	1.00	0.34
ATOM	698	HB2	LEU	48	-7.167	-4.968	-20.385	1.00	0.33
ATOM	699	CG	LEU	48	-8.816	-5.964	-19.434	1.00	0.34
ATOM	700	HG	LEU	48	-8.808	-6.900	-19.972	1.00	0.32
ATOM	701	CD1	LEU	48	-7.952	-6.091	-18.177	1.00	0.41
ATOM	702	HD11	LEU	48	-8.002	-5.171	-17.613	1.00	1.11
ATOM	703	HD12	LEU	48	-6.928	-6.283	-18.462	1.00	1.05
ATOM	704	HD13	LEU	48	-8.315	-6.906	-17.570	1.00	1.15
ATOM	705	CD2	LEU	48	-10.255	-5.628	-19.016	1.00	0.36
ATOM	706	HD21	LEU	48	-10.569	-4.707	-19.478	1.00	1.10
ATOM	707	HD22	LEU	48	-10.299	-5.524	-17.942	1.00	1.09
ATOM	708	HD23	LEU	48	-10.912	-6.428	-19.325	1.00	1.04
ATOM	709	C	LEU	48	-8.289	-3.806	-22.589	1.00	0.25
ATOM	710	O	LEU	48	-7.174	-3.849	-23.071	1.00	0.26
ATOM	711	N	ASN	49	-9.073	-2.775	-22.762	1.00	0.25
ATOM	712	HN	ASN	49	-9.964	-2.770	-22.355	1.00	0.26
ATOM	713	CA	ASN	49	-8.622	-1.604	-23.568	1.00	0.25
ATOM	714	HA	ASN	49	-7.703	-1.842	-24.082	1.00	0.27
ATOM	715	CB	ASN	49	-9.700	-1.245	-24.593	1.00	0.28
ATOM	716	HB1	ASN	49	-9.390	-0.375	-25.153	1.00	0.30
ATOM	717	HB2	ASN	49	-10.628	-1.033	-24.081	1.00	0.28
ATOM	718	CG	ASN	49	-9.902	-2.419	-25.553	1.00	0.32
ATOM	719	OD1	ASN	49	-9.798	-3.564	-25.161	1.00	1.10
ATOM	720	ND2	ASN	49	-10.186	-2.182	-26.804	1.00	1.14
ATOM	721	HD21	ASN	49	-10.268	-1.258	-27.121	1.00	1.94
ATOM	722	HD22	ASN	49	-10.317	-2.927	-27.427	1.00	1.14
ATOM	723	C	ASN	49	-8.391	-0.417	-22.633	1.00	0.24
ATOM	724	O	ASN	49	-9.290	0.016	-21.939	1.00	0.23
ATOM	725	N	PHE	50	-7.192	0.107	-22.606	1.00	0.24
ATOM	726	HN	PHE	50	-6.485	-0.264	-23.173	1.00	0.26
ATOM	727	CA	PHE	50	-6.896	1.263	-21.710	1.00	0.23
ATOM	728	HA	PHE	50	-7.688	1.380	-20.985	1.00	0.21
ATOM	729	CB	PHE	50	-5.574	1.016	-20.981	1.00	0.24
ATOM	730	HB1	PHE	50	-5.357	1.853	-20.334	1.00	0.25
ATOM	731	HB2	PHE	50	-4.780	0.907	-21.705	1.00	0.27
ATOM	732	CG	PHE	50	-5.676	-0.243	-20.154	1.00	0.23

ATOM	733	CD1	PHE	50	-6.266	-0.201	-18.886	1.00	0.25
ATOM	734	HD1	PHE	50	-6.652	0.731	-18.500	1.00	0.28
ATOM	735	CD2	PHE	50	-5.176	-1.451	-20.654	1.00	0.22
ATOM	736	HD2	PHE	50	-4.720	-1.483	-21.633	1.00	0.23
ATOM	737	CE1	PHE	50	-6.358	-1.368	-18.117	1.00	0.25
ATOM	738	HE1	PHE	50	-6.813	-1.336	-17.139	1.00	0.28
ATOM	739	CE2	PHE	50	-5.267	-2.618	-19.886	1.00	0.23
ATOM	740	HE2	PHE	50	-4.881	-3.550	-20.272	1.00	0.25
ATOM	741	CZ	PHE	50	-5.858	-2.576	-18.618	1.00	0.24
ATOM	742	HZ	PHE	50	-5.928	-3.476	-18.025	1.00	0.25
ATOM	743	C	PHE	50	-6.777	2.538	-22.545	1.00	0.26
ATOM	744	O	PHE	50	-6.028	2.596	-23.501	1.00	0.31
ATOM	745	N	THR	51	-7.517	3.555	-22.184	1.00	0.24
ATOM	746	HN	THR	51	-8.109	3.468	-21.413	1.00	0.22
ATOM	747	CA	THR	51	-7.470	4.842	-22.940	1.00	0.27
ATOM	748	HA	THR	51	-6.775	4.762	-23.762	1.00	0.31
ATOM	749	CB	THR	51	-8.868	5.153	-23.483	1.00	0.30
ATOM	750	HB	THR	51	-9.562	5.248	-22.663	1.00	0.29
ATOM	751	OG1	THR	51	-9.283	4.100	-24.341	1.00	0.35
ATOM	752	HG1	THR	51	-9.638	4.491	-25.142	1.00	0.84
ATOM	753	CG2	THR	51	-8.835	6.464	-24.273	1.00	0.34
ATOM	754	HG21	THR	51	-9.805	6.640	-24.716	1.00	1.02
ATOM	755	HG22	THR	51	-8.092	6.394	-25.053	1.00	1.07
ATOM	756	HG23	THR	51	-8.588	7.280	-23.611	1.00	1.13
ATOM	757	C	THR	51	-7.024	5.969	-22.001	1.00	0.25
ATOM	758	O	THR	51	-7.553	6.139	-20.920	1.00	0.22
ATOM	759	N	ARG	52	-6.054	6.740	-22.411	1.00	0.29
ATOM	760	HN	ARG	52	-5.645	6.583	-23.287	1.00	0.32
ATOM	761	CA	ARG	52	-5.566	7.861	-21.556	1.00	0.29
ATOM	762	HA	ARG	52	-5.591	7.563	-20.518	1.00	0.27
ATOM	763	CB	ARG	52	-4.128	8.201	-21.955	1.00	0.35
ATOM	764	HB1	ARG	52	-4.125	8.654	-22.935	1.00	0.39
ATOM	765	HB2	ARG	52	-3.539	7.295	-21.977	1.00	0.38
ATOM	766	CG	ARG	52	-3.521	9.177	-20.945	1.00	0.39
ATOM	767	HG1	ARG	52	-3.645	8.787	-19.946	1.00	0.71
ATOM	768	HG2	ARG	52	-4.017	10.134	-21.025	1.00	0.57
ATOM	769	CD	ARG	52	-2.030	9.345	-21.244	1.00	0.79
ATOM	770	HD1	ARG	52	-1.825	9.001	-22.248	1.00	1.45
ATOM	771	HD2	ARG	52	-1.453	8.763	-20.543	1.00	1.39
ATOM	772	NE	ARG	52	-1.656	10.782	-21.120	1.00	1.47
ATOM	773	HE	ARG	52	-2.354	11.468	-21.073	1.00	2.06
ATOM	774	CZ	ARG	52	-0.398	11.127	-21.071	1.00	2.09
ATOM	775	NH1	ARG	52	-0.070	12.385	-20.960	1.00	3.05
ATOM	776	HH11	ARG	52	-0.782	13.084	-20.911	1.00	3.45
ATOM	777	HH12	ARG	52	0.894	12.649	-20.923	1.00	3.60
ATOM	778	NH2	ARG	52	0.532	10.213	-21.138	1.00	2.31
ATOM	779	HH21	ARG	52	0.281	9.249	-21.226	1.00	2.16
ATOM	780	HH22	ARG	52	1.496	10.477	-21.102	1.00	3.05
ATOM	781	C	ARG	52	-6.460	9.090	-21.758	1.00	0.29
ATOM	782	O	ARG	52	-6.719	9.495	-22.875	1.00	0.33
ATOM	783	N	LEU	53	-6.928	9.689	-20.689	1.00	0.26
ATOM	784	HN	LEU	53	-6.702	9.345	-19.798	1.00	0.25
ATOM	785	CA	LEU	53	-7.803	10.896	-20.822	1.00	0.29
ATOM	786	HA	LEU	53	-8.167	10.972	-21.835	1.00	0.32
ATOM	787	CB	LEU	53	-8.992	10.784	-19.862	1.00	0.28
ATOM	788	HB1	LEU	53	-9.579	11.688	-19.908	1.00	0.31
ATOM	789	HB2	LEU	53	-8.624	10.648	-18.855	1.00	0.28
ATOM	790	CG	LEU	53	-9.866	9.587	-20.249	1.00	0.28
ATOM	791	HG	LEU	53	-9.264	8.690	-20.246	1.00	0.29
ATOM	792	CD1	LEU	53	-10.999	9.440	-19.232	1.00	0.29
ATOM	793	HD11	LEU	53	-11.606	8.585	-19.487	1.00	0.95
ATOM	794	HD12	LEU	53	-11.610	10.331	-19.243	1.00	1.05
ATOM	795	HD13	LEU	53	-10.581	9.303	-18.247	1.00	1.07
ATOM	796	CD2	LEU	53	-10.463	9.799	-21.646	1.00	0.36
ATOM	797	HD21	LEU	53	-10.523	10.856	-21.860	1.00	1.01
ATOM	798	HD22	LEU	53	-11.453	9.370	-21.685	1.00	1.09
ATOM	799	HD23	LEU	53	-9.835	9.319	-22.382	1.00	1.14
ATOM	800	C	LEU	53	-7.000	12.154	-20.483	1.00	0.33
ATOM	801	O	LEU	53	-6.315	12.218	-19.482	1.00	0.34
ATOM	802	N	HIS	54	-7.080	13.154	-21.319	1.00	0.41
ATOM	803	HN	HIS	54	-7.637	13.075	-22.121	1.00	0.45
ATOM	804	CA	HIS	54	-6.324	14.413	-21.062	1.00	0.47
ATOM	805	HA	HIS	54	-5.292	14.183	-20.851	1.00	0.54
ATOM	806	CB	HIS	54	-6.407	15.314	-22.297	1.00	0.60
ATOM	807	HB1	HIS	54	-6.018	16.291	-22.052	1.00	0.64
ATOM	808	HB2	HIS	54	-7.438	15.407	-22.603	1.00	0.61
ATOM	809	CG	HIS	54	-5.602	14.726	-23.426	1.00	0.74

ATOM	810	ND1	HIS	54	-5.645	15.254	-24.707	1.00	1.35
ATOM	811	HD1	HIS	54	-6.172	16.028	-24.996	1.00	1.86
ATOM	812	CD2	HIS	54	-4.740	13.656	-23.493	1.00	0.86
ATOM	813	HD2	HIS	54	-4.480	13.010	-22.668	1.00	1.34
ATOM	814	CE1	HIS	54	-4.834	14.512	-25.481	1.00	1.33
ATOM	815	HE1	HIS	54	-4.670	14.692	-26.533	1.00	1.83
ATOM	816	NE2	HIS	54	-4.257	13.525	-24.792	1.00	0.92
ATOM	817	C	HIS	54	-6.933	15.154	-19.867	1.00	0.43
ATOM	818	O	HIS	54	-6.230	15.714	-19.051	1.00	0.49
ATOM	819	N	ASP	55	-8.236	15.172	-19.767	1.00	0.42
ATOM	820	HN	ASP	55	-8.784	14.719	-20.442	1.00	0.45
ATOM	821	CA	ASP	55	-8.892	15.892	-18.635	1.00	0.49
ATOM	822	HA	ASP	55	-8.217	15.938	-17.796	1.00	0.54
ATOM	823	CB	ASP	55	-9.251	17.314	-19.073	1.00	0.65
ATOM	824	HB1	ASP	55	-9.876	17.774	-18.323	1.00	0.75
ATOM	825	HB2	ASP	55	-9.783	17.277	-20.013	1.00	0.68
ATOM	826	CG	ASP	55	-7.974	18.140	-19.244	1.00	0.71
ATOM	827	OD1	ASP	55	-7.978	19.037	-20.071	1.00	1.19
ATOM	828	OD2	ASP	55	-7.018	17.870	-18.536	1.00	1.28
ATOM	829	C	ASP	55	-10.167	15.156	-18.223	1.00	0.45
ATOM	830	O	ASP	55	-10.638	14.273	-18.912	1.00	0.44
ATOM	831	N	GLY	56	-10.728	15.518	-17.100	1.00	0.46
ATOM	832	HN	GLY	56	-10.328	16.233	-16.563	1.00	0.50
ATOM	833	CA	GLY	56	-11.975	14.848	-16.632	1.00	0.44
ATOM	834	HA1	GLY	56	-12.482	14.399	-17.472	1.00	0.44
ATOM	835	HA2	GLY	56	-12.622	15.579	-16.169	1.00	0.48
ATOM	836	C	GLY	56	-11.624	13.760	-15.614	1.00	0.40
ATOM	837	O	GLY	56	-10.473	13.543	-15.294	1.00	0.42
ATOM	838	N	ILE	57	-12.613	13.078	-15.105	1.00	0.37
ATOM	839	HN	ILE	57	-13.533	13.275	-15.380	1.00	0.39
ATOM	840	CA	ILE	57	-12.352	12.002	-14.106	1.00	0.35
ATOM	841	HA	ILE	57	-11.406	12.184	-13.616	1.00	0.38
ATOM	842	CB	ILE	57	-13.473	12.000	-13.064	1.00	0.41
ATOM	843	HB	ILE	57	-14.415	11.820	-13.561	1.00	0.42
ATOM	844	CG1	ILE	57	-13.508	13.363	-12.360	1.00	0.48
ATOM	845	HG11	ILE	57	-13.512	14.148	-13.101	1.00	0.48
ATOM	846	HG12	ILE	57	-12.631	13.465	-11.737	1.00	0.51
ATOM	847	CG2	ILE	57	-13.216	10.896	-12.037	1.00	0.44
ATOM	848	HG21	ILE	57	-13.315	9.932	-12.513	1.00	1.19
ATOM	849	HG22	ILE	57	-13.934	10.977	-11.235	1.00	1.09
ATOM	850	HG23	ILE	57	-12.218	11.000	-11.639	1.00	1.04
ATOM	851	CD1	ILE	57	-14.765	13.484	-11.488	1.00	0.56
ATOM	852	HD11	ILE	57	-15.459	12.693	-11.728	1.00	1.08
ATOM	853	HD12	ILE	57	-15.235	14.439	-11.668	1.00	1.24
ATOM	854	HD13	ILE	57	-14.487	13.413	-10.447	1.00	1.14
ATOM	855	C	ILE	57	-12.307	10.647	-14.817	1.00	0.30
ATOM	856	O	ILE	57	-13.139	10.353	-15.653	1.00	0.31
ATOM	857	N	ALA	58	-11.337	9.828	-14.493	1.00	0.26
ATOM	858	HN	ALA	58	-10.679	10.096	-13.817	1.00	0.27
ATOM	859	CA	ALA	58	-11.221	8.489	-15.148	1.00	0.23
ATOM	860	HA	ALA	58	-11.957	8.398	-15.932	1.00	0.25
ATOM	861	CB	ALA	58	-9.824	8.339	-15.749	1.00	0.23
ATOM	862	HB1	ALA	58	-9.843	7.585	-16.522	1.00	0.97
ATOM	863	HB2	ALA	58	-9.129	8.044	-14.976	1.00	1.11
ATOM	864	HB3	ALA	58	-9.513	9.280	-16.172	1.00	1.03
ATOM	865	C	ALA	58	-11.443	7.387	-14.114	1.00	0.23
ATOM	866	O	ALA	58	-11.389	7.617	-12.922	1.00	0.27
ATOM	867	N	ASP	59	-11.701	6.189	-14.564	1.00	0.25
ATOM	868	HN	ASP	59	-11.744	6.028	-15.530	1.00	0.28
ATOM	869	CA	ASP	59	-11.934	5.069	-13.613	1.00	0.27
ATOM	870	HA	ASP	59	-12.788	5.296	-12.991	1.00	0.34
ATOM	871	CB	ASP	59	-12.207	3.785	-14.400	1.00	0.33
ATOM	872	HB1	ASP	59	-12.203	2.942	-13.725	1.00	0.34
ATOM	873	HB2	ASP	59	-11.438	3.651	-15.147	1.00	0.32
ATOM	874	CG	ASP	59	-13.572	3.880	-15.084	1.00	0.44
ATOM	875	OD1	ASP	59	-13.791	3.139	-16.028	1.00	1.20
ATOM	876	OD2	ASP	59	-14.374	4.691	-14.653	1.00	1.14
ATOM	877	C	ASP	59	-10.700	4.863	-12.731	1.00	0.22
ATOM	878	O	ASP	59	-10.806	4.767	-11.524	1.00	0.27
ATOM	879	N	ILE	60	-9.534	4.780	-13.326	1.00	0.18
ATOM	880	HN	ILE	60	-9.478	4.850	-14.302	1.00	0.20
ATOM	881	CA	ILE	60	-8.291	4.561	-12.523	1.00	0.22
ATOM	882	HA	ILE	60	-8.554	4.303	-11.512	1.00	0.28
ATOM	883	CB	ILE	60	-7.502	3.404	-13.155	1.00	0.27
ATOM	884	HB	ILE	60	-7.255	3.655	-14.175	1.00	0.28
ATOM	885	CG1	ILE	60	-8.377	2.146	-13.136	1.00	0.30

ATOM	887	HG12	ILE	60	-8.541	1.839	-12.113	1.00	0.36
ATOM	888	CG2	ILE	60	-6.210	3.127	-12.369	1.00	0.39
ATOM	889	HG21	ILE	60	-6.456	2.704	-11.409	1.00	1.05
ATOM	890	HG22	ILE	60	-5.658	4.043	-12.228	1.00	1.10
ATOM	891	HG23	ILE	60	-5.600	2.428	-12.921	1.00	1.12
ATOM	892	CD1	ILE	60	-7.688	1.015	-13.904	1.00	0.38
ATOM	893	HD11	ILE	60	-7.209	1.413	-14.786	1.00	1.07
ATOM	894	HD12	ILE	60	-8.424	0.280	-14.196	1.00	1.14
ATOM	895	HD13	ILE	60	-6.948	0.549	-13.270	1.00	1.04
ATOM	896	C	ILE	60	-7.438	5.834	-12.518	1.00	0.20
ATOM	897	O	ILE	60	-6.731	6.115	-13.464	1.00	0.25
ATOM	898	N	MET	61	-7.473	6.585	-11.448	1.00	0.20
ATOM	899	HN	MET	61	-8.033	6.326	-10.687	1.00	0.25
ATOM	900	CA	MET	61	-6.641	7.822	-11.373	1.00	0.20
ATOM	901	HA	MET	61	-6.327	8.102	-12.366	1.00	0.19
ATOM	902	CB	MET	61	-7.464	8.963	-10.773	1.00	0.24
ATOM	903	HB1	MET	61	-8.331	9.137	-11.392	1.00	0.35
ATOM	904	HB2	MET	61	-6.860	9.856	-10.743	1.00	0.33
ATOM	905	CG	MET	61	-7.918	8.604	-9.358	1.00	0.31
ATOM	906	HG1	MET	61	-7.146	8.870	-8.653	1.00	0.66
ATOM	907	HG2	MET	61	-8.112	7.544	-9.300	1.00	0.67
ATOM	908	SD	MET	61	-9.433	9.519	-8.967	1.00	0.54
ATOM	909	CE	MET	61	-8.878	11.154	-9.516	1.00	0.40
ATOM	910	HE1	MET	61	-9.492	11.914	-9.056	1.00	1.06
ATOM	911	HE2	MET	61	-8.968	11.227	-10.589	1.00	1.16
ATOM	912	HE3	MET	61	-7.846	11.298	-9.232	1.00	1.12
ATOM	913	C	MET	61	-5.396	7.540	-10.524	1.00	0.20
ATOM	914	O	MET	61	-5.478	6.951	-9.463	1.00	0.22
ATOM	915	N	ILE	62	-4.241	7.937	-11.001	1.00	0.20
ATOM	916	HN	ILE	62	-4.207	8.393	-11.868	1.00	0.21
ATOM	917	CA	ILE	62	-2.971	7.678	-10.252	1.00	0.21
ATOM	918	HA	ILE	62	-3.156	6.982	-9.448	1.00	0.20
ATOM	919	CB	ILE	62	-1.938	7.080	-11.211	1.00	0.24
ATOM	920	HB	ILE	62	-1.753	7.781	-12.012	1.00	0.26
ATOM	921	CG1	ILE	62	-2.480	5.762	-11.785	1.00	0.23
ATOM	922	HG11	ILE	62	-3.479	5.922	-12.162	1.00	0.20
ATOM	923	HG12	ILE	62	-2.508	5.018	-11.003	1.00	0.24
ATOM	924	CG2	ILE	62	-0.635	6.812	-10.455	1.00	0.30
ATOM	925	HG21	ILE	62	-0.863	6.443	-9.466	1.00	1.08
ATOM	926	HG22	ILE	62	-0.070	7.729	-10.375	1.00	1.12
ATOM	927	HG23	ILE	62	-0.052	6.076	-10.988	1.00	0.99
ATOM	928	CD1	ILE	62	-1.584	5.262	-12.927	1.00	0.29
ATOM	929	HD11	ILE	62	-0.979	6.073	-13.305	1.00	1.02
ATOM	930	HD12	ILE	62	-2.201	4.876	-13.724	1.00	1.09
ATOM	931	HD13	ILE	62	-0.941	4.476	-12.559	1.00	1.07
ATOM	932	C	ILE	62	-2.423	8.988	-9.677	1.00	0.22
ATOM	933	O	ILE	62	-2.393	10.004	-10.343	1.00	0.27
ATOM	934	N	SER	63	-1.993	8.976	-8.441	1.00	0.20
ATOM	935	HN	SER	63	-2.028	8.147	-7.916	1.00	0.18
ATOM	936	CA	SER	63	-1.452	10.226	-7.829	1.00	0.22
ATOM	937	HA	SER	63	-0.998	10.836	-8.597	1.00	0.26
ATOM	938	CB	SER	63	-2.597	11.000	-7.176	1.00	0.24
ATOM	939	HB1	SER	63	-3.448	11.012	-7.845	1.00	0.25
ATOM	940	HB2	SER	63	-2.286	12.012	-6.978	1.00	0.29
ATOM	941	OG	SER	63	-2.951	10.369	-5.952	1.00	0.25
ATOM	942	HG	SER	63	-3.682	9.772	-6.127	1.00	0.85
ATOM	943	C	SER	63	-0.404	9.879	-6.764	1.00	0.21
ATOM	944	O	SER	63	-0.364	8.775	-6.259	1.00	0.20
ATOM	945	N	PHE	64	0.440	10.823	-6.419	1.00	0.24
ATOM	946	HN	PHE	64	0.380	11.705	-6.841	1.00	0.27
ATOM	947	CA	PHE	64	1.490	10.569	-5.382	1.00	0.24
ATOM	948	HA	PHE	64	1.560	9.511	-5.179	1.00	0.22
ATOM	949	CB	PHE	64	2.840	11.084	-5.895	1.00	0.28
ATOM	950	HB1	PHE	64	3.564	11.047	-5.097	1.00	0.32
ATOM	951	HB2	PHE	64	2.730	12.103	-6.235	1.00	0.32
ATOM	952	CG	PHE	64	3.316	10.220	-7.040	1.00	0.28
ATOM	953	CD1	PHE	64	4.112	9.096	-6.788	1.00	0.30
ATOM	954	HD1	PHE	64	4.385	8.844	-5.774	1.00	0.32
ATOM	955	CD2	PHE	64	2.963	10.545	-8.355	1.00	0.33
ATOM	956	HD2	PHE	64	2.350	11.412	-8.550	1.00	0.37
ATOM	957	CE1	PHE	64	4.553	8.297	-7.850	1.00	0.36
ATOM	958	HE1	PHE	64	5.166	7.430	-7.656	1.00	0.40
ATOM	959	CE2	PHE	64	3.403	9.747	-9.417	1.00	0.40
ATOM	960	HE2	PHE	64	3.130	9.998	-10.431	1.00	0.47
ATOM	961	CZ	PHE	64	4.198	8.623	-9.165	1.00	0.40
ATOM	962	HZ	PHE	64	4.538	8.007	-9.984	1.00	0.47
ATOM	963	C	PHE	64	1.115	11.318	-4.097	1.00	0.27

ATOM	964	O	PHE	64	0.924	12.518	-4.108	1.00	0.36
ATOM	965	N	GLY	65	0.996	10.617	-2.996	1.00	0.30
ATOM	966	HN	GLY	65	1.146	9.649	-3.017	1.00	0.33
ATOM	967	CA	GLY	65	0.615	11.282	-1.709	1.00	0.38
ATOM	968	HA1	GLY	65	-0.152	10.697	-1.224	1.00	0.46
ATOM	969	HA2	GLY	65	0.230	12.270	-1.913	1.00	0.45
ATOM	970	C	GLY	65	1.823	11.397	-0.770	1.00	0.32
ATOM	971	O	GLY	65	2.926	11.007	-1.098	1.00	0.40
ATOM	972	N	ILE	66	1.598	11.926	0.408	1.00	0.30
ATOM	973	HN	ILE	66	0.691	12.220	0.635	1.00	0.36
ATOM	974	CA	ILE	66	2.691	12.081	1.417	1.00	0.36
ATOM	975	HA	ILE	66	3.564	11.534	1.093	1.00	0.40
ATOM	976	CB	ILE	66	3.040	13.564	1.571	1.00	0.41
ATOM	977	HB	ILE	66	2.127	14.134	1.656	1.00	0.64
ATOM	978	CG1	ILE	66	3.829	14.026	0.337	1.00	0.68
ATOM	979	HG11	ILE	66	3.301	13.729	-0.557	1.00	0.95
ATOM	980	HG12	ILE	66	4.804	13.561	0.346	1.00	1.01
ATOM	981	CG2	ILE	66	3.886	13.764	2.831	1.00	0.93
ATOM	982	HG21	ILE	66	4.372	14.727	2.790	1.00	1.50
ATOM	983	HG22	ILE	66	4.632	12.986	2.891	1.00	1.41
ATOM	984	HG23	ILE	66	3.249	13.720	3.702	1.00	1.54
ATOM	985	CD1	ILE	66	3.997	15.551	0.343	1.00	0.70
ATOM	986	HD11	ILE	66	4.944	15.806	0.797	1.00	1.22
ATOM	987	HD12	ILE	66	3.196	16.009	0.902	1.00	1.28
ATOM	988	HD13	ILE	66	3.979	15.917	-0.673	1.00	1.23
ATOM	989	C	ILE	66	2.207	11.519	2.760	1.00	0.46
ATOM	990	O	ILE	66	1.021	11.363	2.958	1.00	0.54
ATOM	991	N	LYS	67	3.129	11.205	3.659	1.00	0.59
ATOM	992	HN	LYS	67	4.073	11.343	3.434	1.00	0.64
ATOM	993	CA	LYS	67	2.780	10.630	5.014	1.00	0.74
ATOM	994	HA	LYS	67	3.072	9.594	5.038	1.00	0.83
ATOM	995	CB	LYS	67	3.550	11.404	6.102	1.00	0.90
ATOM	996	HB1	LYS	67	3.237	12.438	6.089	1.00	0.89
ATOM	997	HB2	LYS	67	4.608	11.352	5.891	1.00	0.96
ATOM	998	CG	LYS	67	3.287	10.815	7.504	1.00	1.08
ATOM	999	HG1	LYS	67	2.254	10.524	7.598	1.00	1.31
ATOM	1000	HG2	LYS	67	3.510	11.565	8.249	1.00	1.33
ATOM	1001	CD	LYS	67	4.179	9.590	7.746	1.00	0.98
ATOM	1002	HD1	LYS	67	5.216	9.885	7.694	1.00	1.07
ATOM	1003	HD2	LYS	67	3.979	8.839	6.999	1.00	1.07
ATOM	1004	CE	LYS	67	3.885	9.016	9.135	1.00	1.17
ATOM	1005	HE1	LYS	67	4.331	8.036	9.220	1.00	1.64
ATOM	1006	HE2	LYS	67	2.817	8.938	9.272	1.00	1.50
ATOM	1007	NZ	LYS	67	4.453	9.913	10.180	1.00	1.93
ATOM	1008	HZ1	LYS	67	4.569	10.870	9.792	1.00	2.38
ATOM	1009	HZ2	LYS	67	5.378	9.547	10.485	1.00	2.43
ATOM	1010	HZ3	LYS	67	3.808	9.948	10.995	1.00	2.40
ATOM	1011	C	LYS	67	1.274	10.732	5.280	1.00	0.72
ATOM	1012	O	LYS	67	0.530	9.804	5.035	1.00	0.79
ATOM	1013	N	GLU	68	0.815	11.855	5.760	1.00	0.77
ATOM	1014	HN	GLU	68	1.425	12.601	5.939	1.00	0.84
ATOM	1015	CA	GLU	68	-0.645	12.004	6.011	1.00	0.84
ATOM	1016	HA	GLU	68	-1.014	11.130	6.530	1.00	0.99
ATOM	1017	CB	GLU	68	-0.895	13.254	6.860	1.00	1.05
ATOM	1018	HB1	GLU	68	-0.393	13.149	7.810	1.00	1.23
ATOM	1019	HB2	GLU	68	-1.956	13.370	7.024	1.00	1.10
ATOM	1020	CG	GLU	68	-0.353	14.487	6.134	1.00	1.15
ATOM	1021	HG1	GLU	68	-1.000	14.730	5.304	1.00	1.32
ATOM	1022	HG2	GLU	68	0.642	14.281	5.768	1.00	1.28
ATOM	1023	CD	GLU	68	-0.308	15.669	7.104	1.00	1.75
ATOM	1024	OE1	GLU	68	0.246	16.692	6.736	1.00	2.45
ATOM	1025	OE2	GLU	68	-0.823	15.530	8.202	1.00	2.16
ATOM	1026	C	GLU	68	-1.346	12.132	4.660	1.00	0.76
ATOM	1027	O	GLU	68	-0.899	12.859	3.795	1.00	1.11
ATOM	1028	N	HIS	69	-2.420	11.414	4.454	1.00	0.94
ATOM	1029	HN	HIS	69	-2.755	10.815	5.155	1.00	1.32
ATOM	1030	CA	HIS	69	-3.114	11.487	3.136	1.00	1.04
ATOM	1031	HA	HIS	69	-2.877	12.437	2.679	1.00	1.25
ATOM	1032	CB	HIS	69	-2.545	10.358	2.243	1.00	1.49
ATOM	1033	HB1	HIS	69	-1.750	9.862	2.783	1.00	2.12
ATOM	1034	HB2	HIS	69	-2.131	10.798	1.351	1.00	2.27
ATOM	1035	CG	HIS	69	-3.570	9.333	1.837	1.00	0.95
ATOM	1036	ND1	HIS	69	-3.818	8.195	2.588	1.00	1.43
ATOM	1037	HD1	HIS	69	-3.415	7.972	3.453	1.00	1.83
ATOM	1038	CD2	HIS	69	-4.355	9.223	0.717	1.00	1.04
ATOM	1039	HD2	HIS	69	-4.403	9.946	-0.082	1.00	1.41
ATOM	1040	CE1	HIS	69	-4.715	7.452	1.912	1.00	1.81

ATOM	1041	HE1	HIS	69	-5.097	6.502	2.257	1.00	2.54
ATOM	1042	NE2	HIS	69	-5.075	8.032	0.765	1.00	1.53
ATOM	1043	C	HIS	69	-4.643	11.435	3.341	1.00	1.14
ATOM	1044	O	HIS	69	-5.392	10.889	2.556	1.00	1.76
ATOM	1045	N	GLY	70	-5.108	12.065	4.393	1.00	1.49
ATOM	1046	HN	GLY	70	-4.487	12.532	4.990	1.00	1.98
ATOM	1047	CA	GLY	70	-6.576	12.123	4.665	1.00	1.86
ATOM	1048	HA1	GLY	70	-7.071	12.633	3.852	1.00	2.28
ATOM	1049	HA2	GLY	70	-6.746	12.667	5.583	1.00	2.09
ATOM	1050	C	GLY	70	-7.155	10.716	4.801	1.00	1.81
ATOM	1051	O	GLY	70	-8.182	10.404	4.232	1.00	2.53
ATOM	1052	N	ASP	71	-6.513	9.863	5.545	1.00	1.55
ATOM	1053	HN	ASP	71	-5.686	10.127	5.999	1.00	1.66
ATOM	1054	CA	ASP	71	-7.047	8.484	5.701	1.00	1.91
ATOM	1055	HA	ASP	71	-8.126	8.513	5.684	1.00	2.42
ATOM	1056	CB	ASP	71	-6.546	7.620	4.546	1.00	2.67
ATOM	1057	HB1	ASP	71	-6.623	6.578	4.813	1.00	3.03
ATOM	1058	HB2	ASP	71	-5.514	7.865	4.341	1.00	2.88
ATOM	1059	CG	ASP	71	-7.397	7.892	3.303	1.00	3.56
ATOM	1060	OD1	ASP	71	-8.476	7.330	3.215	1.00	4.08
ATOM	1061	OD2	ASP	71	-6.960	8.664	2.465	1.00	4.16
ATOM	1062	C	ASP	71	-6.577	7.889	7.028	1.00	1.46
ATOM	1063	O	ASP	71	-5.600	8.323	7.605	1.00	1.78
ATOM	1064	N	PHE	72	-7.260	6.886	7.507	1.00	1.36
ATOM	1065	HN	PHE	72	-8.038	6.546	7.018	1.00	1.67
ATOM	1066	CA	PHE	72	-6.849	6.248	8.786	1.00	1.48
ATOM	1067	HA	PHE	72	-6.504	7.007	9.473	1.00	1.75
ATOM	1068	CB	PHE	72	-8.037	5.503	9.399	1.00	2.01
ATOM	1069	HB1	PHE	72	-8.374	6.028	10.281	1.00	2.58
ATOM	1070	HB2	PHE	72	-7.733	4.503	9.669	1.00	2.43
ATOM	1071	CG	PHE	72	-9.161	5.434	8.395	1.00	2.30
ATOM	1072	CD1	PHE	72	-9.414	4.243	7.704	1.00	2.86
ATOM	1073	HD1	PHE	72	-8.802	3.372	7.887	1.00	3.09
ATOM	1074	CD2	PHE	72	-9.954	6.563	8.158	1.00	2.97
ATOM	1075	HD2	PHE	72	-9.758	7.482	8.691	1.00	3.28
ATOM	1076	CE1	PHE	72	-10.459	4.182	6.775	1.00	3.73
ATOM	1077	HE1	PHE	72	-10.655	3.264	6.242	1.00	4.46
ATOM	1078	CE2	PHE	72	-10.999	6.502	7.229	1.00	3.80
ATOM	1079	HE2	PHE	72	-11.610	7.374	7.045	1.00	4.54
ATOM	1080	CZ	PHE	72	-11.252	5.312	6.537	1.00	4.08
ATOM	1081	HZ	PHE	72	-12.058	5.264	5.821	1.00	4.92
ATOM	1082	C	PHE	72	-5.716	5.266	8.500	1.00	1.41
ATOM	1083	O	PHE	72	-5.384	4.430	9.318	1.00	2.20
ATOM	1084	N	TYR	73	-5.120	5.371	7.338	1.00	1.12
ATOM	1085	HN	TYR	73	-5.412	6.059	6.703	1.00	1.48
ATOM	1086	CA	TYR	73	-3.999	4.457	6.972	1.00	1.25
ATOM	1087	HA	TYR	73	-3.774	3.793	7.790	1.00	1.46
ATOM	1088	CB	TYR	73	-4.391	3.635	5.742	1.00	1.86
ATOM	1089	HB1	TYR	73	-3.531	3.082	5.395	1.00	2.35
ATOM	1090	HB2	TYR	73	-4.726	4.300	4.961	1.00	2.46
ATOM	1091	CG	TYR	73	-5.498	2.670	6.089	1.00	2.08
ATOM	1092	CD1	TYR	73	-5.241	1.585	6.934	1.00	2.58
ATOM	1093	HD1	TYR	73	-4.252	1.444	7.347	1.00	2.82
ATOM	1094	CD2	TYR	73	-6.779	2.853	5.553	1.00	2.85
ATOM	1095	HD2	TYR	73	-6.978	3.691	4.901	1.00	3.24
ATOM	1096	CE1	TYR	73	-6.264	0.683	7.244	1.00	3.48
ATOM	1097	HE1	TYR	73	-6.066	-0.155	7.896	1.00	4.19
ATOM	1098	CE2	TYR	73	-7.802	1.952	5.865	1.00	3.68
ATOM	1099	HE2	TYR	73	-8.789	2.093	5.452	1.00	4.49
ATOM	1100	CZ	TYR	73	-7.545	0.866	6.710	1.00	3.90
ATOM	1101	OH	TYR	73	-8.554	-0.024	7.013	1.00	5.00
ATOM	1102	HH	TYR	73	-8.689	-0.590	6.249	1.00	5.22
ATOM	1103	C	TYR	73	-2.755	5.273	6.609	1.00	0.95
ATOM	1104	O	TYR	73	-2.219	5.127	5.529	1.00	1.21
ATOM	1105	N	PRO	74	-2.273	6.106	7.495	1.00	0.74
ATOM	1106	CA	PRO	74	-1.054	6.895	7.197	1.00	0.82
ATOM	1107	HA	PRO	74	-1.254	7.648	6.453	1.00	1.05
ATOM	1108	CB	PRO	74	-0.746	7.558	8.543	1.00	1.16
ATOM	1109	HB1	PRO	74	-0.786	8.631	8.438	1.00	1.46
ATOM	1110	HB2	PRO	74	0.239	7.261	8.876	1.00	1.28
ATOM	1111	CG	PRO	74	-1.795	7.105	9.566	1.00	1.35
ATOM	1112	HG1	PRO	74	-2.229	7.967	10.049	1.00	1.70
ATOM	1113	HG2	PRO	74	-1.330	6.468	10.305	1.00	1.61
ATOM	1114	CD	PRO	74	-2.889	6.328	8.828	1.00	1.04
ATOM	1115	HD2	PRO	74	-3.098	5.393	9.328	1.00	1.24
ATOM	1116	HD1	PRO	74	-3.778	6.929	8.733	1.00	1.14
ATOM	1117	C	PRO	74	0.097	5.988	6.765	1.00	0.65

ATOM	1118	O	PRO	74	0.136	4.822	7.106	1.00	0.66
ATOM	1119	N	PHE	75	1.038	6.503	6.032	1.00	0.56
ATOM	1120	HN	PHE	75	1.000	7.447	5.770	1.00	0.61
ATOM	1121	CA	PHE	75	2.179	5.651	5.605	1.00	0.45
ATOM	1122	HA	PHE	75	1.816	4.659	5.360	1.00	0.48
ATOM	1123	CB	PHE	75	2.859	6.266	4.379	1.00	0.42
ATOM	1124	HB1	PHE	75	3.761	5.718	4.153	1.00	0.44
ATOM	1125	HB2	PHE	75	3.104	7.298	4.582	1.00	0.45
ATOM	1126	CG	PHE	75	1.915	6.190	3.200	1.00	0.48
ATOM	1127	CD1	PHE	75	1.764	4.986	2.501	1.00	0.41
ATOM	1128	HD1	PHE	75	2.329	4.115	2.797	1.00	0.45
ATOM	1129	CD2	PHE	75	1.184	7.320	2.812	1.00	0.74
ATOM	1130	HD2	PHE	75	1.300	8.249	3.349	1.00	0.90
ATOM	1131	CE1	PHE	75	0.882	4.911	1.415	1.00	0.50
ATOM	1132	HE1	PHE	75	0.767	3.982	0.877	1.00	0.53
ATOM	1133	CE2	PHE	75	0.304	7.245	1.724	1.00	0.85
ATOM	1134	HE2	PHE	75	-0.258	8.117	1.423	1.00	1.09
ATOM	1135	CZ	PHE	75	0.154	6.041	1.026	1.00	0.69
ATOM	1136	HZ	PHE	75	-0.526	5.983	0.188	1.00	0.80
ATOM	1137	C	PHE	75	3.159	5.561	6.776	1.00	0.43
ATOM	1138	O	PHE	75	3.111	6.360	7.690	1.00	0.50
ATOM	1139	N	ASP	76	4.020	4.582	6.782	1.00	0.37
ATOM	1140	HN	ASP	76	4.028	3.929	6.050	1.00	0.32
ATOM	1141	CA	ASP	76	4.967	4.432	7.927	1.00	0.43
ATOM	1142	HA	ASP	76	4.551	4.906	8.804	1.00	0.50
ATOM	1143	CB	ASP	76	5.180	2.946	8.215	1.00	0.46
ATOM	1144	HB1	ASP	76	4.224	2.467	8.365	1.00	0.49
ATOM	1145	HB2	ASP	76	5.784	2.834	9.104	1.00	0.54
ATOM	1146	CG	ASP	76	5.892	2.295	7.028	1.00	0.38
ATOM	1147	OD1	ASP	76	6.468	1.236	7.218	1.00	0.45
ATOM	1148	OD2	ASP	76	5.846	2.864	5.950	1.00	0.30
ATOM	1149	C	ASP	76	6.314	5.074	7.596	1.00	0.42
ATOM	1150	O	ASP	76	7.314	4.770	8.216	1.00	0.54
ATOM	1151	N	GLY	77	6.347	5.958	6.632	1.00	0.35
ATOM	1152	HN	GLY	77	5.525	6.187	6.151	1.00	0.36
ATOM	1153	CA	GLY	77	7.634	6.625	6.267	1.00	0.38
ATOM	1154	HA1	GLY	77	8.378	6.388	7.004	1.00	0.45
ATOM	1155	HA2	GLY	77	7.484	7.696	6.238	1.00	0.44
ATOM	1156	C	GLY	77	8.084	6.131	4.884	1.00	0.31
ATOM	1157	O	GLY	77	7.262	5.767	4.068	1.00	0.37
ATOM	1158	N	PRO	78	9.370	6.117	4.603	1.00	0.33
ATOM	1159	CA	PRO	78	9.856	5.651	3.274	1.00	0.36
ATOM	1160	HA	PRO	78	9.435	6.254	2.488	1.00	0.42
ATOM	1161	CB	PRO	78	11.364	5.903	3.359	1.00	0.46
ATOM	1162	HB1	PRO	78	11.671	6.542	2.545	1.00	0.56
ATOM	1163	HB2	PRO	78	11.892	4.962	3.303	1.00	0.48
ATOM	1164	CG	PRO	78	11.675	6.592	4.694	1.00	0.64
ATOM	1165	HG1	PRO	78	11.965	7.616	4.516	1.00	0.87
ATOM	1166	HG2	PRO	78	12.478	6.068	5.194	1.00	0.83
ATOM	1167	CD	PRO	78	10.418	6.562	5.563	1.00	0.45
ATOM	1168	HD2	PRO	78	10.535	5.848	6.369	1.00	0.48
ATOM	1169	HD1	PRO	78	10.187	7.544	5.944	1.00	0.49
ATOM	1170	C	PRO	78	9.564	4.165	3.027	1.00	0.30
ATOM	1171	O	PRO	78	8.860	3.808	2.105	1.00	0.28
ATOM	1172	N	SER	79	10.102	3.297	3.840	1.00	0.31
ATOM	1173	HN	SER	79	10.670	3.604	4.577	1.00	0.35
ATOM	1174	CA	SER	79	9.855	1.837	3.647	1.00	0.30
ATOM	1175	HA	SER	79	9.916	1.599	2.595	1.00	0.30
ATOM	1176	CB	SER	79	10.911	1.037	4.410	1.00	0.37
ATOM	1177	HB1	SER	79	11.888	1.465	4.225	1.00	0.42
ATOM	1178	HB2	SER	79	10.901	0.013	4.076	1.00	0.39
ATOM	1179	OG	SER	79	10.617	1.080	5.800	1.00	0.38
ATOM	1180	HG	SER	79	11.173	1.752	6.201	1.00	0.98
ATOM	1181	C	SER	79	8.463	1.470	4.173	1.00	0.27
ATOM	1182	O	SER	79	7.888	2.183	4.971	1.00	0.25
ATOM	1183	N	GLY	80	7.927	0.356	3.734	1.00	0.31
ATOM	1184	HN	GLY	80	8.420	-0.200	3.095	1.00	0.37
ATOM	1185	CA	GLY	80	6.576	-0.081	4.207	1.00	0.30
ATOM	1186	HA1	GLY	80	6.224	0.586	4.977	1.00	0.31
ATOM	1187	HA2	GLY	80	6.646	-1.083	4.607	1.00	0.36
ATOM	1188	C	GLY	80	5.584	-0.070	3.042	1.00	0.25
ATOM	1189	O	GLY	80	5.850	-0.601	1.981	1.00	0.25
ATOM	1190	N	LEU	81	4.440	0.531	3.232	1.00	0.23
ATOM	1191	HN	LEU	81	4.246	0.951	4.096	1.00	0.25
ATOM	1192	CA	LEU	81	3.428	0.577	2.138	1.00	0.21
ATOM	1193	HA	LEU	81	3.259	-0.417	1.761	1.00	0.22
ATOM	1194	CB	LEU	81	2.123	1.164	2.692	1.00	0.24

ATOM	1195	HB1	LEU	81	1.587	1.658	1.896	1.00	0.25
ATOM	1196	HB2	LEU	81	2.356	1.881	3.465	1.00	0.29
ATOM	1197	CG	LEU	81	1.240	0.058	3.283	1.00	0.28
ATOM	1198	HG	LEU	81	1.856	-0.678	3.779	1.00	0.31
ATOM	1199	CD1	LEU	81	0.265	0.680	4.285	1.00	0.33
ATOM	1200	HD11	LEU	81	0.071	1.706	4.009	1.00	1.05
ATOM	1201	HD12	LEU	81	0.696	0.649	5.274	1.00	1.10
ATOM	1202	HD13	LEU	81	-0.662	0.125	4.278	1.00	1.06
ATOM	1203	CD2	LEU	81	0.426	-0.606	2.168	1.00	0.31
ATOM	1204	HD21	LEU	81	1.087	-0.997	1.412	1.00	1.02
ATOM	1205	HD22	LEU	81	-0.233	0.126	1.724	1.00	1.09
ATOM	1206	HD23	LEU	81	-0.161	-1.411	2.584	1.00	1.06
ATOM	1207	C	LEU	81	3.953	1.475	1.017	1.00	0.20
ATOM	1208	O	LEU	81	3.988	2.679	1.141	1.00	0.22
ATOM	1209	N	LEU	82	4.366	0.899	-0.078	1.00	0.18
ATOM	1210	HN	LEU	82	4.334	-0.077	-0.162	1.00	0.18
ATOM	1211	CA	LEU	82	4.901	1.728	-1.195	1.00	0.18
ATOM	1212	HA	LEU	82	5.519	2.520	-0.799	1.00	0.19
ATOM	1213	CB	LEU	82	5.728	0.840	-2.128	1.00	0.18
ATOM	1214	HB1	LEU	82	6.235	1.457	-2.854	1.00	0.20
ATOM	1215	HB2	LEU	82	5.071	0.151	-2.640	1.00	0.20
ATOM	1216	CG	LEU	82	6.763	0.050	-1.323	1.00	0.18
ATOM	1217	HG	LEU	82	6.262	-0.523	-0.556	1.00	0.22
ATOM	1218	CD1	LEU	82	7.513	-0.898	-2.259	1.00	0.17
ATOM	1219	HD11	LEU	82	8.102	-0.321	-2.957	1.00	0.97
ATOM	1220	HD12	LEU	82	6.802	-1.503	-2.802	1.00	0.95
ATOM	1221	HD13	LEU	82	8.163	-1.537	-1.681	1.00	0.98
ATOM	1222	CD2	LEU	82	7.764	1.010	-0.675	1.00	0.23
ATOM	1223	HD21	LEU	82	8.019	1.790	-1.375	1.00	1.03
ATOM	1224	HD22	LEU	82	8.657	0.466	-0.403	1.00	1.07
ATOM	1225	HD23	LEU	82	7.326	1.447	0.209	1.00	1.02
ATOM	1226	C	LEU	82	3.740	2.329	-1.986	1.00	0.19
ATOM	1227	O	LEU	82	3.882	3.341	-2.646	1.00	0.21
ATOM	1228	N	ALA	83	2.594	1.711	-1.919	1.00	0.21
ATOM	1229	HN	ALA	83	2.512	0.899	-1.376	1.00	0.24
ATOM	1230	CA	ALA	83	1.410	2.225	-2.662	1.00	0.22
ATOM	1231	HA	ALA	83	1.217	3.251	-2.381	1.00	0.22
ATOM	1232	CB	ALA	83	1.668	2.140	-4.171	1.00	0.23
ATOM	1233	HB1	ALA	83	2.522	2.746	-4.429	1.00	0.98
ATOM	1234	HB2	ALA	83	0.801	2.497	-4.705	1.00	1.00
ATOM	1235	HB3	ALA	83	1.860	1.113	-4.445	1.00	1.05
ATOM	1236	C	ALA	83	0.204	1.350	-2.317	1.00	0.27
ATOM	1237	O	ALA	83	0.342	0.301	-1.720	1.00	0.36
ATOM	1238	N	HIS	84	-0.976	1.762	-2.686	1.00	0.24
ATOM	1239	HN	HIS	84	-1.075	2.609	-3.170	1.00	0.20
ATOM	1240	CA	HIS	84	-2.173	0.933	-2.370	1.00	0.30
ATOM	1241	HA	HIS	84	-1.940	-0.108	-2.542	1.00	0.36
ATOM	1242	CB	HIS	84	-2.562	1.127	-0.903	1.00	0.40
ATOM	1243	HB1	HIS	84	-1.695	0.965	-0.278	1.00	0.48
ATOM	1244	HB2	HIS	84	-3.332	0.419	-0.638	1.00	0.45
ATOM	1245	CG	HIS	84	-3.074	2.525	-0.692	1.00	0.44
ATOM	1246	ND1	HIS	84	-4.384	2.781	-0.321	1.00	1.32
ATOM	1247	HD1	HIS	84	-5.084	2.112	-0.169	1.00	2.02
ATOM	1248	CD2	HIS	84	-2.465	3.752	-0.788	1.00	0.74
ATOM	1249	HD2	HIS	84	-1.432	3.915	-1.060	1.00	1.58
ATOM	1250	CE1	HIS	84	-4.521	4.114	-0.208	1.00	1.21
ATOM	1251	HE1	HIS	84	-5.441	4.606	0.071	1.00	1.87
ATOM	1252	NE2	HIS	84	-3.381	4.754	-0.482	1.00	0.53
ATOM	1253	C	HIS	84	-3.337	1.343	-3.274	1.00	0.25
ATOM	1254	O	HIS	84	-3.347	2.417	-3.843	1.00	0.23
ATOM	1255	N	ALA	85	-4.313	0.489	-3.417	1.00	0.27
ATOM	1256	HN	ALA	85	-4.279	-0.374	-2.954	1.00	0.34
ATOM	1257	CA	ALA	85	-5.474	0.817	-4.291	1.00	0.24
ATOM	1258	HA	ALA	85	-5.582	1.890	-4.364	1.00	0.22
ATOM	1259	CB	ALA	85	-5.236	0.231	-5.685	1.00	0.25
ATOM	1260	HB1	ALA	85	-5.079	-0.835	-5.605	1.00	1.05
ATOM	1261	HB2	ALA	85	-4.364	0.690	-6.126	1.00	1.05
ATOM	1262	HB3	ALA	85	-6.097	0.420	-6.308	1.00	1.06
ATOM	1263	C	ALA	85	-6.748	0.210	-3.698	1.00	0.26
ATOM	1264	O	ALA	85	-6.694	-0.611	-2.804	1.00	0.33
ATOM	1265	N	PHE	86	-7.892	0.605	-4.198	1.00	0.28
ATOM	1266	HN	PHE	86	-7.905	1.264	-4.922	1.00	0.31
ATOM	1267	CA	PHE	86	-9.179	0.053	-3.677	1.00	0.34
ATOM	1268	HA	PHE	86	-9.000	-0.443	-2.737	1.00	0.39
ATOM	1269	CB	PHE	86	-10.170	1.205	-3.471	1.00	0.36
ATOM	1270	HB1	PHE	86	-11.177	0.821	-3.459	1.00	0.42
ATOM	1271	HB2	PHE	86	-10.068	1.913	-4.279	1.00	0.33

ATOM	1272	CG	PHE	86	-9.877	1.896	-2.159	1.00	0.39
ATOM	1273	CD1	PHE	86	-8.784	2.764	-2.050	1.00	0.46
ATOM	1274	HD1	PHE	86	-8.146	2.939	-2.903	1.00	0.67
ATOM	1275	CD2	PHE	86	-10.703	1.670	-1.051	1.00	0.67
ATOM	1276	HD2	PHE	86	-11.546	1.001	-1.133	1.00	0.91
ATOM	1277	CE1	PHE	86	-8.516	3.406	-0.835	1.00	0.50
ATOM	1278	HE1	PHE	86	-7.673	4.075	-0.751	1.00	0.69
ATOM	1279	CE2	PHE	86	-10.435	2.311	0.165	1.00	0.74
ATOM	1280	HE2	PHE	86	-11.071	2.136	1.020	1.00	1.02
ATOM	1281	CZ	PHE	86	-9.342	3.179	0.273	1.00	0.54
ATOM	1282	HZ	PHE	86	-9.135	3.674	1.211	1.00	0.62
ATOM	1283	C	PHE	86	-9.746	-0.940	-4.710	1.00	0.36
ATOM	1284	O	PHE	86	-9.480	-0.812	-5.889	1.00	0.34
ATOM	1285	N	PRO	87	-10.516	-1.926	-4.293	1.00	0.43
ATOM	1286	CA	PRO	87	-11.082	-2.914	-5.257	1.00	0.46
ATOM	1287	HA	PRO	87	-10.296	-3.524	-5.665	1.00	0.53
ATOM	1288	CB	PRO	87	-11.990	-3.770	-4.370	1.00	0.60
ATOM	1289	HB1	PRO	87	-11.644	-4.792	-4.377	1.00	0.69
ATOM	1290	HB2	PRO	87	-13.004	-3.727	-4.742	1.00	0.73
ATOM	1291	CG	PRO	87	-11.943	-3.225	-2.937	1.00	0.58
ATOM	1292	HG1	PRO	87	-11.694	-4.022	-2.253	1.00	0.61
ATOM	1293	HG2	PRO	87	-12.905	-2.808	-2.676	1.00	0.66
ATOM	1294	CD	PRO	87	-10.872	-2.135	-2.861	1.00	0.50
ATOM	1295	HD2	PRO	87	-11.277	-1.235	-2.421	1.00	0.50
ATOM	1296	HD1	PRO	87	-10.014	-2.484	-2.309	1.00	0.52
ATOM	1297	C	PRO	87	-11.895	-2.246	-6.379	1.00	0.40
ATOM	1298	O	PRO	87	-12.221	-1.078	-6.299	1.00	0.42
ATOM	1299	N	PRO	88	-12.221	-2.981	-7.419	1.00	0.44
ATOM	1300	CA	PRO	88	-13.007	-2.416	-8.554	1.00	0.48
ATOM	1301	HA	PRO	88	-12.443	-1.645	-9.053	1.00	0.52
ATOM	1302	CB	PRO	88	-13.163	-3.622	-9.488	1.00	0.61
ATOM	1303	HB1	PRO	88	-12.604	-3.449	-10.395	1.00	0.83
ATOM	1304	HB2	PRO	88	-14.204	-3.772	-9.728	1.00	0.74
ATOM	1305	CG	PRO	88	-12.609	-4.863	-8.781	1.00	0.57
ATOM	1306	HG1	PRO	88	-11.945	-5.395	-9.446	1.00	0.71
ATOM	1307	HG2	PRO	88	-13.425	-5.508	-8.488	1.00	0.64
ATOM	1308	CD	PRO	88	-11.835	-4.413	-7.540	1.00	0.56
ATOM	1309	HD2	PRO	88	-12.146	-4.977	-6.671	1.00	0.62
ATOM	1310	HD1	PRO	88	-10.773	-4.503	-7.702	1.00	0.65
ATOM	1311	C	PRO	88	-14.372	-1.873	-8.109	1.00	0.47
ATOM	1312	O	PRO	88	-15.380	-2.551	-8.172	1.00	0.88
ATOM	1313	N	GLY	89	-14.400	-0.647	-7.661	1.00	0.63
ATOM	1314	HN	GLY	89	-13.571	-0.129	-7.626	1.00	1.01
ATOM	1315	CA	GLY	89	-15.681	-0.026	-7.209	1.00	0.65
ATOM	1316	HA1	GLY	89	-15.536	0.422	-6.239	1.00	0.62
ATOM	1317	HA2	GLY	89	-16.455	-0.778	-7.148	1.00	0.78
ATOM	1318	C	GLY	89	-16.092	1.057	-8.210	1.00	0.74
ATOM	1319	O	GLY	89	-15.541	1.151	-9.289	1.00	0.84
ATOM	1320	N	PRO	90	-17.044	1.878	-7.852	1.00	0.95
ATOM	1321	CA	PRO	90	-17.499	2.973	-8.750	1.00	1.19
ATOM	1322	HA	PRO	90	-17.819	2.565	-9.697	1.00	1.37
ATOM	1323	CB	PRO	90	-18.720	3.532	-7.990	1.00	1.55
ATOM	1324	HB1	PRO	90	-19.602	3.432	-8.605	1.00	1.85
ATOM	1325	HB2	PRO	90	-18.572	4.567	-7.740	1.00	1.74
ATOM	1326	CG	PRO	90	-18.913	2.724	-6.702	1.00	1.46
ATOM	1327	HG1	PRO	90	-19.828	2.155	-6.763	1.00	1.60
ATOM	1328	HG2	PRO	90	-18.959	3.396	-5.857	1.00	1.57
ATOM	1329	CD	PRO	90	-17.729	1.769	-6.539	1.00	1.17
ATOM	1330	HD2	PRO	90	-17.083	2.099	-5.736	1.00	1.17
ATOM	1331	HD1	PRO	90	-18.067	0.759	-6.375	1.00	1.28
ATOM	1332	C	PRO	90	-16.375	4.011	-8.972	1.00	1.14
ATOM	1333	O	PRO	90	-15.269	3.649	-9.320	1.00	1.53
ATOM	1334	N	ASN	91	-16.624	5.282	-8.790	1.00	1.17
ATOM	1335	HN	ASN	91	-17.514	5.578	-8.517	1.00	1.40
ATOM	1336	CA	ASN	91	-15.541	6.286	-9.008	1.00	1.38
ATOM	1337	HA	ASN	91	-15.147	6.169	-10.005	1.00	1.58
ATOM	1338	CB	ASN	91	-16.116	7.700	-8.857	1.00	1.87
ATOM	1339	HB1	ASN	91	-15.336	8.372	-8.532	1.00	2.33
ATOM	1340	HB2	ASN	91	-16.908	7.686	-8.122	1.00	1.96
ATOM	1341	CG	ASN	91	-16.678	8.184	-10.197	1.00	2.69
ATOM	1342	OD1	ASN	91	-16.132	7.890	-11.242	1.00	3.20
ATOM	1343	ND2	ASN	91	-17.748	8.931	-10.212	1.00	3.47
ATOM	1344	HD21	ASN	91	-18.186	9.176	-9.370	1.00	3.59
ATOM	1345	HD22	ASN	91	-18.112	9.249	-11.064	1.00	4.20
ATOM	1346	C	ASN	91	-14.404	6.098	-7.992	1.00	1.15
ATOM	1347	O	ASN	91	-13.242	6.135	-8.344	1.00	1.26
ATOM	1348	N	TYR	92	-14.719	5.924	-6.735	1.00	1.01

ATOM	1349	HN	TYR	92	-15.660	5.916	-6.462	1.00	1.08
ATOM	1350	CA	TYR	92	-13.639	5.768	-5.711	1.00	0.97
ATOM	1351	HA	TYR	92	-12.994	6.632	-5.739	1.00	1.14
ATOM	1352	CB	TYR	92	-14.262	5.652	-4.319	1.00	1.09
ATOM	1353	HB1	TYR	92	-13.543	5.214	-3.643	1.00	1.62
ATOM	1354	HB2	TYR	92	-15.135	5.020	-4.369	1.00	1.45
ATOM	1355	CG	TYR	92	-14.656	7.018	-3.810	1.00	1.52
ATOM	1356	CD1	TYR	92	-13.672	7.979	-3.549	1.00	2.14
ATOM	1357	HD1	TYR	92	-12.631	7.747	-3.719	1.00	2.46
ATOM	1358	CD2	TYR	92	-16.006	7.320	-3.588	1.00	2.44
ATOM	1359	HD2	TYR	92	-16.766	6.580	-3.789	1.00	2.86
ATOM	1360	CE1	TYR	92	-14.037	9.241	-3.066	1.00	3.06
ATOM	1361	HE1	TYR	92	-13.278	9.982	-2.865	1.00	3.78
ATOM	1362	CE2	TYR	92	-16.370	8.582	-3.107	1.00	3.33
ATOM	1363	HE2	TYR	92	-17.411	8.815	-2.936	1.00	4.19
ATOM	1364	CZ	TYR	92	-15.386	9.542	-2.846	1.00	3.50
ATOM	1365	OH	TYR	92	-15.746	10.786	-2.368	1.00	4.57
ATOM	1366	HH	TYR	92	-15.602	10.791	-1.419	1.00	4.91
ATOM	1367	C	TYR	92	-12.808	4.508	-5.966	1.00	0.78
ATOM	1368	O	TYR	92	-11.605	4.506	-5.798	1.00	0.81
ATOM	1369	N	GLY	93	-13.436	3.430	-6.337	1.00	0.64
ATOM	1370	HN	GLY	93	-14.410	3.441	-6.445	1.00	0.70
ATOM	1371	CA	GLY	93	-12.674	2.170	-6.560	1.00	0.51
ATOM	1372	HA1	GLY	93	-13.366	1.366	-6.740	1.00	0.51
ATOM	1373	HA2	GLY	93	-12.090	1.947	-5.678	1.00	0.51
ATOM	1374	C	GLY	93	-11.739	2.310	-7.761	1.00	0.49
ATOM	1375	O	GLY	93	-11.832	3.242	-8.534	1.00	0.61
ATOM	1376	N	GLY	94	-10.844	1.373	-7.923	1.00	0.45
ATOM	1377	HN	GLY	94	-10.799	0.627	-7.288	1.00	0.44
ATOM	1378	CA	GLY	94	-9.902	1.420	-9.075	1.00	0.55
ATOM	1379	HA1	GLY	94	-10.459	1.569	-9.988	1.00	0.63
ATOM	1380	HA2	GLY	94	-9.363	0.485	-9.133	1.00	0.58
ATOM	1381	C	GLY	94	-8.905	2.569	-8.901	1.00	0.60
ATOM	1382	O	GLY	94	-8.109	2.838	-9.772	1.00	1.14
ATOM	1383	N	ASP	95	-8.933	3.252	-7.790	1.00	0.24
ATOM	1384	HN	ASP	95	-9.581	3.028	-7.089	1.00	0.52
ATOM	1385	CA	ASP	95	-7.976	4.382	-7.597	1.00	0.24
ATOM	1386	HA	ASP	95	-7.888	4.939	-8.518	1.00	0.28
ATOM	1387	CB	ASP	95	-8.493	5.303	-6.491	1.00	0.26
ATOM	1388	HB1	ASP	95	-9.500	5.617	-6.724	1.00	0.28
ATOM	1389	HB2	ASP	95	-7.853	6.170	-6.415	1.00	0.30
ATOM	1390	CG	ASP	95	-8.494	4.549	-5.162	1.00	0.28
ATOM	1391	OD1	ASP	95	-8.543	5.200	-4.132	1.00	1.08
ATOM	1392	OD2	ASP	95	-8.440	3.331	-5.198	1.00	1.14
ATOM	1393	C	ASP	95	-6.605	3.827	-7.202	1.00	0.23
ATOM	1394	O	ASP	95	-6.479	2.683	-6.815	1.00	0.24
ATOM	1395	N	ALA	96	-5.573	4.626	-7.297	1.00	0.23
ATOM	1396	HN	ALA	96	-5.692	5.546	-7.614	1.00	0.23
ATOM	1397	CA	ALA	96	-4.215	4.131	-6.926	1.00	0.25
ATOM	1398	HA	ALA	96	-4.307	3.360	-6.175	1.00	0.25
ATOM	1399	CB	ALA	96	-3.527	3.553	-8.164	1.00	0.30
ATOM	1400	HB1	ALA	96	-2.528	3.236	-7.905	1.00	1.08
ATOM	1401	HB2	ALA	96	-3.476	4.309	-8.934	1.00	1.08
ATOM	1402	HB3	ALA	96	-4.090	2.706	-8.528	1.00	1.03
ATOM	1403	C	ALA	96	-3.375	5.284	-6.372	1.00	0.25
ATOM	1404	O	ALA	96	-3.222	6.313	-7.005	1.00	0.29
ATOM	1405	N	HXS	97	-2.831	5.113	-5.192	1.00	0.25
ATOM	1406	HN	HXS	97	-2.976	4.271	-4.710	1.00	0.28
ATOM	1407	CA	HXS	97	-1.996	6.187	-4.574	1.00	0.27
ATOM	1408	HA	HXS	97	-2.010	7.068	-5.198	1.00	0.28
ATOM	1409	CB	HXS	97	-2.564	6.537	-3.197	1.00	0.33
ATOM	1410	HB1	HXS	97	-1.969	7.319	-2.750	1.00	0.44
ATOM	1411	HB2	HXS	97	-2.540	5.661	-2.566	1.00	0.39
ATOM	1412	CG	HXS	97	-3.983	7.009	-3.349	1.00	0.37
ATOM	1413	ND1	HXS	97	-4.697	7.052	-2.163	1.00	0.80
ATOM	1414	CD2	HXS	97	-4.783	7.420	-4.384	1.00	0.55
ATOM	1415	HD2	HXS	97	-4.517	7.497	-5.428	1.00	0.94
ATOM	1416	CE1	HXS	97	-5.919	7.497	-2.499	1.00	0.86
ATOM	1417	HE1	HXS	97	-6.724	7.632	-1.795	1.00	1.24
ATOM	1418	NE2	HXS	97	-6.018	7.722	-3.819	1.00	0.59
ATOM	1419	HE2	HXS	97	-6.812	8.044	-4.294	1.00	0.72
ATOM	1420	C	HXS	97	-0.552	5.700	-4.420	1.00	0.26
ATOM	1421	O	HXS	97	-0.299	4.525	-4.237	1.00	0.39
ATOM	1422	N	PHE	98	0.391	6.604	-4.496	1.00	0.18
ATOM	1423	HN	PHE	98	0.147	7.540	-4.648	1.00	0.23
ATOM	1424	CA	PHE	98	1.832	6.230	-4.360	1.00	0.17
ATOM	1425	HA	PHE	98	1.921	5.190	-4.085	1.00	0.18

ATOM	1426	CB	PHE	98	2.543	6.472	-5.691	1.00	0.18
ATOM	1427	HB1	PHE	98	3.611	6.464	-5.536	1.00	0.21
ATOM	1428	HB2	PHE	98	2.243	7.431	-6.085	1.00	0.20
ATOM	1429	CG	PHE	98	2.169	5.391	-6.674	1.00	0.19
ATOM	1430	CD1	PHE	98	3.114	4.428	-7.048	1.00	0.22
ATOM	1431	HD1	PHE	98	4.110	4.456	-6.631	1.00	0.25
ATOM	1432	CD2	PHE	98	0.880	5.355	-7.214	1.00	0.22
ATOM	1433	HD2	PHE	98	0.151	6.098	-6.924	1.00	0.24
ATOM	1434	CE1	PHE	98	2.768	3.429	-7.963	1.00	0.25
ATOM	1435	HE1	PHE	98	3.496	2.685	-8.252	1.00	0.29
ATOM	1436	CE2	PHE	98	0.533	4.355	-8.127	1.00	0.26
ATOM	1437	HE2	PHE	98	-0.462	4.327	-8.542	1.00	0.31
ATOM	1438	CZ	PHE	98	1.478	3.392	-8.503	1.00	0.26
ATOM	1439	HZ	PHE	98	1.214	2.622	-9.211	1.00	0.30
ATOM	1440	C	PHE	98	2.487	7.104	-3.286	1.00	0.17
ATOM	1441	O	PHE	98	2.081	8.226	-3.058	1.00	0.19
ATOM	1442	N	ASP	99	3.498	6.604	-2.625	1.00	0.19
ATOM	1443	HN	ASP	99	3.813	5.693	-2.820	1.00	0.22
ATOM	1444	CA	ASP	99	4.167	7.424	-1.570	1.00	0.20
ATOM	1445	HA	ASP	99	3.421	7.956	-0.998	1.00	0.20
ATOM	1446	CB	ASP	99	4.973	6.516	-0.638	1.00	0.25
ATOM	1447	HB1	ASP	99	5.567	7.122	0.029	1.00	0.28
ATOM	1448	HB2	ASP	99	5.624	5.884	-1.226	1.00	0.30
ATOM	1449	CG	ASP	99	4.023	5.646	0.180	1.00	0.41
ATOM	1450	OD1	ASP	99	2.838	5.680	-0.100	1.00	0.89
ATOM	1451	OD2	ASP	99	4.497	4.968	1.079	1.00	0.27
ATOM	1452	C	ASP	99	5.123	8.426	-2.224	1.00	0.21
ATOM	1453	O	ASP	99	6.020	8.054	-2.954	1.00	0.25
ATOM	1454	N	ASP	100	4.946	9.694	-1.962	1.00	0.23
ATOM	1455	HN	ASP	100	4.222	9.976	-1.365	1.00	0.23
ATOM	1456	CA	ASP	100	5.857	10.710	-2.565	1.00	0.29
ATOM	1457	HA	ASP	100	6.169	10.379	-3.545	1.00	0.31
ATOM	1458	CB	ASP	100	5.127	12.049	-2.684	1.00	0.34
ATOM	1459	HB1	ASP	100	5.130	12.544	-1.727	1.00	0.34
ATOM	1460	HB2	ASP	100	4.109	11.879	-2.999	1.00	0.34
ATOM	1461	CG	ASP	100	5.844	12.929	-3.710	1.00	0.43
ATOM	1462	OD1	ASP	100	5.240	13.887	-4.164	1.00	1.21
ATOM	1463	OD2	ASP	100	6.984	12.630	-4.025	1.00	1.12
ATOM	1464	C	ASP	100	7.085	10.885	-1.667	1.00	0.30
ATOM	1465	O	ASP	100	8.032	11.559	-2.018	1.00	0.32
ATOM	1466	N	ASP	101	7.074	10.280	-0.510	1.00	0.31
ATOM	1467	HN	ASP	101	6.298	9.741	-0.249	1.00	0.32
ATOM	1468	CA	ASP	101	8.236	10.407	0.415	1.00	0.33
ATOM	1469	HA	ASP	101	8.647	11.403	0.345	1.00	0.36
ATOM	1470	CB	ASP	101	7.778	10.142	1.851	1.00	0.39
ATOM	1471	HB1	ASP	101	8.641	10.060	2.495	1.00	0.41
ATOM	1472	HB2	ASP	101	7.216	9.220	1.884	1.00	0.39
ATOM	1473	CG	ASP	101	6.896	11.296	2.330	1.00	0.45
ATOM	1474	OD1	ASP	101	7.027	12.380	1.786	1.00	1.25
ATOM	1475	OD2	ASP	101	6.104	11.076	3.231	1.00	1.09
ATOM	1476	C	ASP	101	9.304	9.385	0.028	1.00	0.30
ATOM	1477	O	ASP	101	10.411	9.405	0.529	1.00	0.29
ATOM	1478	N	GLU	102	8.971	8.484	-0.849	1.00	0.30
ATOM	1479	HN	GLU	102	8.068	8.484	-1.230	1.00	0.31
ATOM	1480	CA	GLU	102	9.950	7.444	-1.266	1.00	0.29
ATOM	1481	HA	GLU	102	10.649	7.263	-0.463	1.00	0.30
ATOM	1482	CB	GLU	102	9.195	6.155	-1.585	1.00	0.35
ATOM	1483	HB1	GLU	102	9.873	5.437	-2.020	1.00	0.36
ATOM	1484	HB2	GLU	102	8.397	6.368	-2.282	1.00	0.40
ATOM	1485	CG	GLU	102	8.611	5.584	-0.293	1.00	0.46
ATOM	1486	HG1	GLU	102	8.020	6.342	0.200	1.00	1.18
ATOM	1487	HG2	GLU	102	9.415	5.276	0.356	1.00	1.03
ATOM	1488	CD	GLU	102	7.724	4.381	-0.616	1.00	0.83
ATOM	1489	OE1	GLU	102	7.601	4.060	-1.786	1.00	1.63
ATOM	1490	OE2	GLU	102	7.184	3.801	0.314	1.00	0.87
ATOM	1491	C	GLU	102	10.707	7.917	-2.508	1.00	0.25
ATOM	1492	O	GLU	102	10.359	8.910	-3.115	1.00	0.25
ATOM	1493	N	THR	103	11.741	7.213	-2.886	1.00	0.25
ATOM	1494	HN	THR	103	12.003	6.416	-2.379	1.00	0.28
ATOM	1495	CA	THR	103	12.525	7.620	-4.088	1.00	0.23
ATOM	1496	HA	THR	103	12.356	8.665	-4.301	1.00	0.23
ATOM	1497	CB	THR	103	14.016	7.383	-3.824	1.00	0.27
ATOM	1498	HB	THR	103	14.169	6.359	-3.521	1.00	0.30
ATOM	1499	OG1	THR	103	14.455	8.252	-2.789	1.00	0.29
ATOM	1500	HG1	THR	103	15.334	8.564	-3.016	1.00	0.86
ATOM	1501	CG2	THR	103	14.820	7.656	-5.098	1.00	0.29
ATOM	1502	HG21	THR	103	15.864	7.777	-4.846	1.00	1.08

ATOM	1503	HG22	THR	103	14.457	8.557	-5.569	1.00	1.08
ATOM	1504	HG23	THR	103	14.710	6.824	-5.779	1.00	1.01
ATOM	1505	C	THR	103	12.083	6.777	-5.281	1.00	0.22
ATOM	1506	O	THR	103	12.417	5.614	-5.394	1.00	0.23
ATOM	1507	N	TRP	104	11.332	7.358	-6.175	1.00	0.21
ATOM	1508	HN	TRP	104	11.076	8.297	-6.063	1.00	0.23
ATOM	1509	CA	TRP	104	10.867	6.598	-7.364	1.00	0.21
ATOM	1510	HA	TRP	104	10.750	5.556	-7.104	1.00	0.20
ATOM	1511	CB	TRP	104	9.525	7.165	-7.831	1.00	0.23
ATOM	1512	HB1	TRP	104	9.188	6.623	-8.702	1.00	0.24
ATOM	1513	HB2	TRP	104	9.641	8.210	-8.078	1.00	0.25
ATOM	1514	CG	TRP	104	8.520	7.018	-6.731	1.00	0.24
ATOM	1515	CD1	TRP	104	8.098	8.019	-5.924	1.00	0.31
ATOM	1516	HD1	TRP	104	8.427	9.045	-5.972	1.00	0.36
ATOM	1517	CD2	TRP	104	7.811	5.821	-6.300	1.00	0.21
ATOM	1518	NE1	TRP	104	7.176	7.512	-5.026	1.00	0.31
ATOM	1519	HE1	TRP	104	6.718	8.030	-4.331	1.00	0.36
ATOM	1520	CE2	TRP	104	6.963	6.162	-5.220	1.00	0.24
ATOM	1521	CE3	TRP	104	7.819	4.486	-6.739	1.00	0.18
ATOM	1522	HE3	TRP	104	8.458	4.198	-7.559	1.00	0.19
ATOM	1523	CZ2	TRP	104	6.153	5.213	-4.596	1.00	0.23
ATOM	1524	HZ2	TRP	104	5.515	5.499	-3.774	1.00	0.27
ATOM	1525	CZ3	TRP	104	7.005	3.527	-6.114	1.00	0.20
ATOM	1526	HZ3	TRP	104	7.019	2.504	-6.460	1.00	0.23
ATOM	1527	CH2	TRP	104	6.173	3.891	-5.045	1.00	0.21
ATOM	1528	HH2	TRP	104	5.548	3.150	-4.568	1.00	0.23
ATOM	1529	C	TRP	104	11.911	6.732	-8.474	1.00	0.21
ATOM	1530	O	TRP	104	12.276	7.824	-8.864	1.00	0.24
ATOM	1531	N	THR	105	12.403	5.630	-8.973	1.00	0.20
ATOM	1532	HN	THR	105	12.098	4.763	-8.633	1.00	0.19
ATOM	1533	CA	THR	105	13.437	5.685	-10.048	1.00	0.21
ATOM	1534	HA	THR	105	13.415	6.652	-10.525	1.00	0.24
ATOM	1535	CB	THR	105	14.817	5.459	-9.428	1.00	0.21
ATOM	1536	HB	THR	105	15.018	6.233	-8.704	1.00	0.21
ATOM	1537	OG1	THR	105	15.806	5.497	-10.447	1.00	0.24
ATOM	1538	HG1	THR	105	15.882	6.404	-10.752	1.00	0.86
ATOM	1539	CG2	THR	105	14.846	4.101	-8.729	1.00	0.21
ATOM	1540	HG21	THR	105	15.178	4.233	-7.711	1.00	1.04
ATOM	1541	HG22	THR	105	15.524	3.442	-9.249	1.00	1.07
ATOM	1542	HG23	THR	105	13.854	3.674	-8.731	1.00	0.99
ATOM	1543	C	THR	105	13.166	4.597	-11.087	1.00	0.23
ATOM	1544	O	THR	105	12.521	3.606	-10.808	1.00	0.23
ATOM	1545	N	SER	106	13.668	4.769	-12.282	1.00	0.26
ATOM	1546	HN	SER	106	14.194	5.572	-12.480	1.00	0.29
ATOM	1547	CA	SER	106	13.454	3.739	-13.337	1.00	0.29
ATOM	1548	HA	SER	106	12.570	3.163	-13.111	1.00	0.30
ATOM	1549	CB	SER	106	13.290	4.423	-14.695	1.00	0.35
ATOM	1550	HB1	SER	106	14.249	4.467	-15.193	1.00	1.09
ATOM	1551	HB2	SER	106	12.916	5.424	-14.554	1.00	0.96
ATOM	1552	OG	SER	106	12.365	3.685	-15.483	1.00	1.44
ATOM	1553	HG	SER	106	11.671	4.285	-15.766	1.00	1.97
ATOM	1554	C	SER	106	14.674	2.817	-13.372	1.00	0.28
ATOM	1555	O	SER	106	14.669	1.781	-14.006	1.00	0.31
ATOM	1556	N	SER	107	15.715	3.187	-12.677	1.00	0.26
ATOM	1557	HN	SER	107	15.687	4.023	-12.166	1.00	0.25
ATOM	1558	CA	SER	107	16.940	2.340	-12.641	1.00	0.27
ATOM	1559	HA	SER	107	17.018	1.778	-13.560	1.00	0.29
ATOM	1560	CB	SER	107	18.175	3.226	-12.474	1.00	0.28
ATOM	1561	HB1	SER	107	18.292	3.847	-13.353	1.00	1.12
ATOM	1562	HB2	SER	107	19.049	2.609	-12.355	1.00	1.04
ATOM	1563	OG	SER	107	18.017	4.040	-11.320	1.00	1.29
ATOM	1564	HG	SER	107	18.556	4.827	-11.436	1.00	1.82
ATOM	1565	C	SER	107	16.836	1.376	-11.460	1.00	0.26
ATOM	1566	O	SER	107	15.829	1.324	-10.781	1.00	0.26
ATOM	1567	N	SER	108	17.859	0.609	-11.203	1.00	0.28
ATOM	1568	HN	SER	108	18.666	0.658	-11.757	1.00	0.31
ATOM	1569	CA	SER	108	17.788	-0.342	-10.061	1.00	0.30
ATOM	1570	HA	SER	108	16.775	-0.706	-9.967	1.00	0.30
ATOM	1571	CB	SER	108	18.728	-1.527	-10.330	1.00	0.36
ATOM	1572	HB1	SER	108	19.561	-1.505	-9.642	1.00	1.09
ATOM	1573	HB2	SER	108	19.103	-1.468	-11.338	1.00	0.95
ATOM	1574	OG	SER	108	18.005	-2.741	-10.176	1.00	1.47
ATOM	1575	HG	SER	108	18.550	-3.456	-10.513	1.00	2.00
ATOM	1576	C	SER	108	18.181	0.390	-8.767	1.00	0.28
ATOM	1577	O	SER	108	19.279	0.265	-8.261	1.00	0.33
ATOM	1578	N	LYS	109	17.272	1.157	-8.224	1.00	0.24
ATOM	1579	HN	LYS	109	16.392	1.241	-8.646	1.00	0.23

ATOM	1580	CA	LYS	109	17.561	1.897	-6.960	1.00	0.23
ATOM	1581	HA	LYS	109	18.275	1.341	-6.370	1.00	0.25
ATOM	1582	CB	LYS	109	18.123	3.293	-7.268	1.00	0.24
ATOM	1583	HB1	LYS	109	18.172	3.868	-6.355	1.00	0.27
ATOM	1584	HB2	LYS	109	17.472	3.793	-7.970	1.00	0.25
ATOM	1585	CG	LYS	109	19.525	3.177	-7.868	1.00	0.30
ATOM	1586	HG1	LYS	109	19.476	2.615	-8.785	1.00	0.54
ATOM	1587	HG2	LYS	109	20.177	2.675	-7.170	1.00	0.70
ATOM	1588	CD	LYS	109	20.072	4.574	-8.169	1.00	0.75
ATOM	1589	HD1	LYS	109	20.124	5.144	-7.254	1.00	1.27
ATOM	1590	HD2	LYS	109	19.420	5.074	-8.870	1.00	1.27
ATOM	1591	CE	LYS	109	21.475	4.453	-8.770	1.00	1.13
ATOM	1592	HE1	LYS	109	21.396	4.264	-9.830	1.00	1.68
ATOM	1593	HE2	LYS	109	22.000	3.636	-8.297	1.00	1.68
ATOM	1594	NZ	LYS	109	22.224	5.721	-8.545	1.00	1.79
ATOM	1595	HZ1	LYS	109	21.689	6.516	-8.948	1.00	2.22
ATOM	1596	HZ2	LYS	109	23.155	5.660	-9.006	1.00	2.17
ATOM	1597	HZ3	LYS	109	22.351	5.873	-7.525	1.00	2.34
ATOM	1598	C	LYS	109	16.259	2.052	-6.175	1.00	0.21
ATOM	1599	O	LYS	109	15.190	2.110	-6.747	1.00	0.20
ATOM	1600	N	GLY	110	16.338	2.124	-4.873	1.00	0.23
ATOM	1601	HN	GLY	110	17.212	2.079	-4.432	1.00	0.26
ATOM	1602	CA	GLY	110	15.099	2.283	-4.056	1.00	0.22
ATOM	1603	HA1	GLY	110	14.751	3.302	-4.124	1.00	0.23
ATOM	1604	HA2	GLY	110	15.316	2.044	-3.024	1.00	0.25
ATOM	1605	C	GLY	110	14.013	1.342	-4.581	1.00	0.19
ATOM	1606	O	GLY	110	14.281	0.216	-4.949	1.00	0.20
ATOM	1607	N	TYR	111	12.789	1.801	-4.626	1.00	0.17
ATOM	1608	HN	TYR	111	12.599	2.716	-4.330	1.00	0.18
ATOM	1609	CA	TYR	111	11.683	0.941	-5.136	1.00	0.15
ATOM	1610	HA	TYR	111	11.975	-0.098	-5.088	1.00	0.16
ATOM	1611	CB	TYR	111	10.437	1.162	-4.277	1.00	0.15
ATOM	1612	HB1	TYR	111	9.633	0.540	-4.641	1.00	0.15
ATOM	1613	HB2	TYR	111	10.143	2.200	-4.330	1.00	0.16
ATOM	1614	CG	TYR	111	10.745	0.798	-2.844	1.00	0.17
ATOM	1615	CD1	TYR	111	10.648	-0.533	-2.422	1.00	0.17
ATOM	1616	HD1	TYR	111	10.354	-1.301	-3.121	1.00	0.17
ATOM	1617	CD2	TYR	111	11.127	1.794	-1.936	1.00	0.20
ATOM	1618	HD2	TYR	111	11.201	2.821	-2.261	1.00	0.23
ATOM	1619	CE1	TYR	111	10.933	-0.868	-1.093	1.00	0.19
ATOM	1620	HE1	TYR	111	10.858	-1.895	-0.767	1.00	0.20
ATOM	1621	CE2	TYR	111	11.412	1.459	-0.607	1.00	0.22
ATOM	1622	HE2	TYR	111	11.706	2.227	0.093	1.00	0.26
ATOM	1623	CZ	TYR	111	11.315	0.127	-0.185	1.00	0.21
ATOM	1624	OH	TYR	111	11.595	-0.204	1.125	1.00	0.23
ATOM	1625	HH	TYR	111	12.543	-0.121	1.255	1.00	0.95
ATOM	1626	C	TYR	111	11.374	1.321	-6.588	1.00	0.14
ATOM	1627	O	TYR	111	10.949	2.424	-6.871	1.00	0.15
ATOM	1628	N	ASN	112	11.581	0.421	-7.511	1.00	0.15
ATOM	1629	HN	ASN	112	11.924	-0.464	-7.264	1.00	0.17
ATOM	1630	CA	ASN	112	11.295	0.739	-8.939	1.00	0.16
ATOM	1631	HA	ASN	112	11.870	1.605	-9.235	1.00	0.16
ATOM	1632	CB	ASN	112	11.677	-0.450	-9.822	1.00	0.19
ATOM	1633	HB1	ASN	112	11.025	-1.276	-9.607	1.00	0.22
ATOM	1634	HB2	ASN	112	12.698	-0.739	-9.622	1.00	0.19
ATOM	1635	CG	ASN	112	11.531	-0.060	-11.295	1.00	0.24
ATOM	1636	OD1	ASN	112	10.446	0.248	-11.748	1.00	0.96
ATOM	1637	ND2	ASN	112	12.583	-0.059	-12.067	1.00	1.06
ATOM	1638	HD21	ASN	112	13.458	-0.308	-11.704	1.00	1.80
ATOM	1639	HD22	ASN	112	12.497	0.189	-13.012	1.00	1.08
ATOM	1640	C	ASN	112	9.803	1.040	-9.108	1.00	0.15
ATOM	1641	O	ASN	112	8.953	0.310	-8.637	1.00	0.14
ATOM	1642	N	LEU	113	9.482	2.112	-9.777	1.00	0.15
ATOM	1643	HN	LEU	113	10.187	2.684	-10.145	1.00	0.16
ATOM	1644	CA	LEU	113	8.049	2.475	-9.984	1.00	0.15
ATOM	1645	HA	LEU	113	7.582	2.620	-9.025	1.00	0.14
ATOM	1646	CB	LEU	113	7.981	3.781	-10.791	1.00	0.16
ATOM	1647	HB1	LEU	113	8.513	3.646	-11.721	1.00	0.17
ATOM	1648	HB2	LEU	113	8.452	4.571	-10.226	1.00	0.16
ATOM	1649	CG	LEU	113	6.523	4.177	-11.095	1.00	0.17
ATOM	1650	HG	LEU	113	6.041	3.387	-11.652	1.00	0.18
ATOM	1651	CD1	LEU	113	5.748	4.421	-9.793	1.00	0.18
ATOM	1652	HD11	LEU	113	4.841	4.969	-10.007	1.00	0.99
ATOM	1653	HD12	LEU	113	6.359	4.991	-9.110	1.00	1.00
ATOM	1654	HD13	LEU	113	5.490	3.474	-9.343	1.00	0.97
ATOM	1655	CD2	LEU	113	6.526	5.457	-11.943	1.00	0.20
ATOM	1656	HD21	LEU	113	6.115	6.277	-11.324	1.00	1.06

ATOM	1657	HD22	LEU	113	5.930	5.302	-12.830	1.00	1.03
ATOM	1658	HD23	LEU	113	7.539	5.696	-12.231	1.00	1.00
ATOM	1659	C	LEU	113	7.320	1.361	-10.743	1.00	0.15
ATOM	1660	O	LEU	113	6.203	1.014	-10.419	1.00	0.15
ATOM	1661	N	PHE	114	7.928	0.817	-11.762	1.00	0.16
ATOM	1662	HN	PHE	114	8.822	1.123	-12.020	1.00	0.17
ATOM	1663	CA	PHE	114	7.245	-0.250	-12.555	1.00	0.17
ATOM	1664	HA	PHE	114	6.338	0.151	-12.980	1.00	0.18
ATOM	1665	CB	PHE	114	8.159	-0.720	-13.685	1.00	0.21
ATOM	1666	HB1	PHE	114	9.077	-1.108	-13.271	1.00	0.22
ATOM	1667	HB2	PHE	114	8.380	0.111	-14.340	1.00	0.22
ATOM	1668	CG	PHE	114	7.457	-1.807	-14.464	1.00	0.24
ATOM	1669	CD1	PHE	114	7.545	-3.135	-14.031	1.00	0.35
ATOM	1670	HD1	PHE	114	8.105	-3.376	-13.147	1.00	0.43
ATOM	1671	CD2	PHE	114	6.724	-1.494	-15.613	1.00	0.24
ATOM	1672	HD2	PHE	114	6.655	-0.470	-15.950	1.00	0.28
ATOM	1673	CE1	PHE	114	6.902	-4.149	-14.741	1.00	0.39
ATOM	1674	HE1	PHE	114	6.975	-5.171	-14.402	1.00	0.50
ATOM	1675	CE2	PHE	114	6.078	-2.512	-16.327	1.00	0.26
ATOM	1676	HE2	PHE	114	5.511	-2.273	-17.214	1.00	0.30
ATOM	1677	CZ	PHE	114	6.168	-3.839	-15.890	1.00	0.32
ATOM	1678	HZ	PHE	114	5.670	-4.623	-16.438	1.00	0.35
ATOM	1679	C	PHE	114	6.900	-1.452	-11.676	1.00	0.17
ATOM	1680	O	PHE	114	5.842	-2.034	-11.806	1.00	0.17
ATOM	1681	N	LEU	115	7.774	-1.846	-10.797	1.00	0.18
ATOM	1682	HN	LEU	115	8.631	-1.380	-10.706	1.00	0.18
ATOM	1683	CA	LEU	115	7.463	-3.028	-9.946	1.00	0.20
ATOM	1684	HA	LEU	115	7.297	-3.882	-10.579	1.00	0.21
ATOM	1685	CB	LEU	115	8.634	-3.304	-8.984	1.00	0.23
ATOM	1686	HB1	LEU	115	8.237	-3.650	-8.041	1.00	0.26
ATOM	1687	HB2	LEU	115	9.172	-2.387	-8.821	1.00	0.22
ATOM	1688	CG	LEU	115	9.612	-4.369	-9.539	1.00	0.28
ATOM	1689	HG	LEU	115	10.397	-4.525	-8.812	1.00	0.33
ATOM	1690	CD1	LEU	115	8.886	-5.702	-9.749	1.00	0.36
ATOM	1691	HD11	LEU	115	9.551	-6.514	-9.498	1.00	0.99
ATOM	1692	HD12	LEU	115	8.578	-5.795	-10.779	1.00	1.11
ATOM	1693	HD13	LEU	115	8.017	-5.740	-9.109	1.00	1.13
ATOM	1694	CD2	LEU	115	10.249	-3.903	-10.859	1.00	0.30
ATOM	1695	HD21	LEU	115	10.497	-4.761	-11.466	1.00	1.10
ATOM	1696	HD22	LEU	115	11.149	-3.351	-10.645	1.00	1.06
ATOM	1697	HD23	LEU	115	9.567	-3.272	-11.395	1.00	1.01
ATOM	1698	C	LEU	115	6.194	-2.748	-9.136	1.00	0.19
ATOM	1699	O	LEU	115	5.280	-3.548	-9.106	1.00	0.20
ATOM	1700	N	VAL	116	6.130	-1.624	-8.475	1.00	0.18
ATOM	1701	HN	VAL	116	6.879	-0.993	-8.508	1.00	0.18
ATOM	1702	CA	VAL	116	4.919	-1.305	-7.664	1.00	0.19
ATOM	1703	HA	VAL	116	4.686	-2.146	-7.028	1.00	0.21
ATOM	1704	CB	VAL	116	5.203	-0.078	-6.794	1.00	0.20
ATOM	1705	HB	VAL	116	5.581	0.722	-7.414	1.00	0.19
ATOM	1706	CG1	VAL	116	3.914	0.381	-6.103	1.00	0.22
ATOM	1707	HG11	VAL	116	3.253	0.832	-6.828	1.00	1.05
ATOM	1708	HG12	VAL	116	4.155	1.105	-5.339	1.00	1.05
ATOM	1709	HG13	VAL	116	3.426	-0.470	-5.650	1.00	1.03
ATOM	1710	CG2	VAL	116	6.246	-0.443	-5.737	1.00	0.21
ATOM	1711	HG21	VAL	116	7.188	-0.654	-6.221	1.00	1.02
ATOM	1712	HG22	VAL	116	5.917	-1.317	-5.194	1.00	0.98
ATOM	1713	HG23	VAL	116	6.370	0.382	-5.052	1.00	1.03
ATOM	1714	C	VAL	116	3.724	-1.020	-8.582	1.00	0.18
ATOM	1715	O	VAL	116	2.615	-1.433	-8.312	1.00	0.19
ATOM	1716	N	ALA	117	3.934	-0.307	-9.659	1.00	0.17
ATOM	1717	HN	ALA	117	4.833	0.028	-9.859	1.00	0.16
ATOM	1718	CA	ALA	117	2.796	0.007	-10.572	1.00	0.17
ATOM	1719	HA	ALA	117	2.064	0.598	-10.044	1.00	0.19
ATOM	1720	CB	ALA	117	3.306	0.795	-11.780	1.00	0.18
ATOM	1721	HB1	ALA	117	4.378	0.709	-11.840	1.00	1.05
ATOM	1722	HB2	ALA	117	3.033	1.834	-11.674	1.00	1.01
ATOM	1723	HB3	ALA	117	2.863	0.397	-12.682	1.00	0.98
ATOM	1724	C	ALA	117	2.150	-1.291	-11.058	1.00	0.17
ATOM	1725	O	ALA	117	0.956	-1.480	-10.951	1.00	0.19
ATOM	1726	N	ALA	118	2.931	-2.187	-11.588	1.00	0.16
ATOM	1727	HN	ALA	118	3.893	-2.015	-11.663	1.00	0.16
ATOM	1728	CA	ALA	118	2.366	-3.472	-12.083	1.00	0.17
ATOM	1729	HA	ALA	118	1.643	-3.273	-12.859	1.00	0.19
ATOM	1730	CB	ALA	118	3.491	-4.335	-12.653	1.00	0.17
ATOM	1731	HB1	ALA	118	3.125	-5.338	-12.812	1.00	1.05
ATOM	1732	HB2	ALA	118	4.316	-4.358	-11.956	1.00	1.02
ATOM	1733	HB3	ALA	118	3.824	-3.920	-13.583	1.00	1.03

ATOM	1734	C	ALA	118	1.687	-4.220	-10.935	1.00	0.17
ATOM	1735	O	ALA	118	0.699	-4.901	-11.124	1.00	0.18
ATOM	1736	N	HIS	119	2.225	-4.123	-9.751	1.00	0.16
ATOM	1737	HN	HIS	119	3.035	-3.585	-9.623	1.00	0.16
ATOM	1738	CA	HIS	119	1.627	-4.855	-8.599	1.00	0.17
ATOM	1739	HA	HIS	119	1.576	-5.907	-8.833	1.00	0.18
ATOM	1740	CB	HIS	119	2.513	-4.655	-7.368	1.00	0.19
ATOM	1741	HB1	HIS	119	2.547	-3.605	-7.116	1.00	0.19
ATOM	1742	HB2	HIS	119	3.512	-5.005	-7.584	1.00	0.20
ATOM	1743	CG	HIS	119	1.950	-5.431	-6.210	1.00	0.21
ATOM	1744	ND1	HIS	119	2.228	-6.775	-6.020	1.00	0.26
ATOM	1745	HD1	HIS	119	2.791	-7.336	-6.593	1.00	0.30
ATOM	1746	CD2	HIS	119	1.128	-5.067	-5.172	1.00	0.20
ATOM	1747	HD2	HIS	119	0.719	-4.079	-5.019	1.00	0.21
ATOM	1748	CE1	HIS	119	1.585	-7.168	-4.906	1.00	0.27
ATOM	1749	HE1	HIS	119	1.622	-8.171	-4.509	1.00	0.33
ATOM	1750	NE2	HIS	119	0.899	-6.166	-4.350	1.00	0.23
ATOM	1751	C	HIS	119	0.215	-4.333	-8.299	1.00	0.17
ATOM	1752	O	HIS	119	-0.721	-5.101	-8.185	1.00	0.18
ATOM	1753	N	GLU	120	0.043	-3.044	-8.160	1.00	0.18
ATOM	1754	HN	GLU	120	0.801	-2.430	-8.248	1.00	0.18
ATOM	1755	CA	GLU	120	-1.322	-2.520	-7.860	1.00	0.20
ATOM	1756	HA	GLU	120	-1.666	-2.977	-6.943	1.00	0.21
ATOM	1757	CB	GLU	120	-1.294	-0.999	-7.668	1.00	0.22
ATOM	1758	HB1	GLU	120	-0.719	-0.763	-6.785	1.00	0.37
ATOM	1759	HB2	GLU	120	-2.302	-0.635	-7.542	1.00	0.33
ATOM	1760	CG	GLU	120	-0.663	-0.314	-8.875	1.00	0.41
ATOM	1761	HG1	GLU	120	-1.125	-0.668	-9.781	1.00	0.63
ATOM	1762	HG2	GLU	120	0.393	-0.531	-8.895	1.00	0.87
ATOM	1763	CD	GLU	120	-0.875	1.194	-8.757	1.00	0.94
ATOM	1764	OE1	GLU	120	-0.757	1.703	-7.654	1.00	1.67
ATOM	1765	OE2	GLU	120	-1.151	1.816	-9.769	1.00	1.56
ATOM	1766	C	GLU	120	-2.291	-2.903	-8.984	1.00	0.20
ATOM	1767	O	GLU	120	-3.432	-3.238	-8.737	1.00	0.21
ATOM	1768	N	PHE	121	-1.853	-2.872	-10.217	1.00	0.19
ATOM	1769	HN	PHE	121	-0.928	-2.608	-10.405	1.00	0.19
ATOM	1770	CA	PHE	121	-2.767	-3.251	-11.331	1.00	0.21
ATOM	1771	HA	PHE	121	-3.628	-2.600	-11.317	1.00	0.23
ATOM	1772	CB	PHE	121	-2.053	-3.130	-12.685	1.00	0.22
ATOM	1773	HB1	PHE	121	-2.576	-3.726	-13.419	1.00	0.24
ATOM	1774	HB2	PHE	121	-1.041	-3.493	-12.587	1.00	0.21
ATOM	1775	CG	PHE	121	-2.026	-1.684	-13.141	1.00	0.25
ATOM	1776	CD1	PHE	121	-0.804	-1.019	-13.308	1.00	0.27
ATOM	1777	HD1	PHE	121	0.121	-1.535	-13.113	1.00	0.40
ATOM	1778	CD2	PHE	121	-3.227	-1.007	-13.403	1.00	0.45
ATOM	1779	HD2	PHE	121	-4.173	-1.513	-13.281	1.00	0.60
ATOM	1780	CE1	PHE	121	-0.781	0.314	-13.733	1.00	0.29
ATOM	1781	HE1	PHE	121	0.163	0.824	-13.862	1.00	0.39
ATOM	1782	CE2	PHE	121	-3.202	0.327	-13.828	1.00	0.49
ATOM	1783	HE2	PHE	121	-4.127	0.847	-14.029	1.00	0.68
ATOM	1784	CZ	PHE	121	-1.979	0.988	-13.993	1.00	0.34
ATOM	1785	HZ	PHE	121	-1.961	2.017	-14.321	1.00	0.38
ATOM	1786	C	PHE	121	-3.228	-4.693	-11.120	1.00	0.20
ATOM	1787	O	PHE	121	-4.374	-5.027	-11.344	1.00	0.21
ATOM	1788	N	GLY	122	-2.344	-5.551	-10.690	1.00	0.18
ATOM	1789	HN	GLY	122	-1.424	-5.262	-10.514	1.00	0.17
ATOM	1790	CA	GLY	122	-2.737	-6.970	-10.464	1.00	0.20
ATOM	1791	HA1	GLY	122	-1.890	-7.523	-10.092	1.00	0.21
ATOM	1792	HA2	GLY	122	-3.072	-7.404	-11.394	1.00	0.21
ATOM	1793	C	GLY	122	-3.867	-7.022	-9.435	1.00	0.20
ATOM	1794	O	GLY	122	-4.823	-7.756	-9.589	1.00	0.22
ATOM	1795	N	HIS	123	-3.778	-6.240	-8.392	1.00	0.20
ATOM	1796	HN	HIS	123	-3.005	-5.644	-8.287	1.00	0.20
ATOM	1797	CA	HIS	123	-4.864	-6.243	-7.371	1.00	0.22
ATOM	1798	HA	HIS	123	-5.047	-7.255	-7.042	1.00	0.23
ATOM	1799	CB	HIS	123	-4.456	-5.382	-6.174	1.00	0.25
ATOM	1800	HB1	HIS	123	-5.324	-5.180	-5.564	1.00	0.30
ATOM	1801	HB2	HIS	123	-4.041	-4.449	-6.527	1.00	0.25
ATOM	1802	CG	HIS	123	-3.427	-6.108	-5.354	1.00	0.27
ATOM	1803	ND1	HIS	123	-3.736	-7.247	-4.628	1.00	0.37
ATOM	1804	HD1	HIS	123	-4.611	-7.685	-4.581	1.00	0.45
ATOM	1805	CD2	HIS	123	-2.096	-5.866	-5.125	1.00	0.25
ATOM	1806	HD2	HIS	123	-1.532	-5.046	-5.545	1.00	0.27
ATOM	1807	CE1	HIS	123	-2.614	-7.644	-4.001	1.00	0.38
ATOM	1808	HE1	HIS	123	-2.553	-8.514	-3.367	1.00	0.47
ATOM	1809	NE2	HIS	123	-1.584	-6.837	-4.269	1.00	0.29
ATOM	1810	C	HIS	123	-6.137	-5.671	-7.883	1.00	0.23

ATOM	1811	O	HIS	123	-7.229	-6.148	-7.755	1.00	0.25
ATOM	1812	N	SER	124	-6.002	-4.646	-8.788	1.00	0.23
ATOM	1813	HN	SER	124	-5.110	-4.278	-8.962	1.00	0.22
ATOM	1814	CA	SER	124	-7.196	-4.030	-9.429	1.00	0.25
ATOM	1815	HA	SER	124	-7.928	-3.790	-8.672	1.00	0.27
ATOM	1816	CB	SER	124	-6.778	-2.751	-10.156	1.00	0.27
ATOM	1817	HB1	SER	124	-6.219	-2.119	-9.478	1.00	0.29
ATOM	1818	HB2	SER	124	-7.654	-2.224	-10.494	1.00	0.29
ATOM	1819	OG	SER	124	-5.975	-3.091	-11.279	1.00	0.25
ATOM	1820	HG	SER	124	-6.545	-3.131	-12.050	1.00	0.88
ATOM	1821	C	SER	124	-7.805	-5.006	-10.437	1.00	0.24
ATOM	1822	O	SER	124	-8.975	-4.932	-10.755	1.00	0.26
ATOM	1823	N	LEU	125	-7.022	-5.913	-10.952	1.00	0.22
ATOM	1824	HN	LEU	125	-6.078	-5.953	-10.690	1.00	0.21
ATOM	1825	CA	LEU	125	-7.562	-6.879	-11.949	1.00	0.23
ATOM	1826	HA	LEU	125	-8.285	-6.374	-12.568	1.00	0.24
ATOM	1827	CB	LEU	125	-6.420	-7.398	-12.827	1.00	0.22
ATOM	1828	HB1	LEU	125	-6.759	-8.247	-13.398	1.00	0.24
ATOM	1829	HB2	LEU	125	-5.594	-7.698	-12.197	1.00	0.22
ATOM	1830	CG	LEU	125	-5.956	-6.280	-13.779	1.00	0.22
ATOM	1831	HG	LEU	125	-5.928	-5.343	-13.241	1.00	0.24
ATOM	1832	CD1	LEU	125	-4.556	-6.601	-14.302	1.00	0.25
ATOM	1833	HD11	LEU	125	-4.588	-7.515	-14.874	1.00	0.99
ATOM	1834	HD12	LEU	125	-3.879	-6.719	-13.471	1.00	1.00
ATOM	1835	HD13	LEU	125	-4.215	-5.794	-14.933	1.00	1.05
ATOM	1836	CD2	LEU	125	-6.913	-6.155	-14.976	1.00	0.24
ATOM	1837	HD21	LEU	125	-7.793	-5.604	-14.682	1.00	1.05
ATOM	1838	HD22	LEU	125	-7.201	-7.135	-15.324	1.00	1.00
ATOM	1839	HD23	LEU	125	-6.415	-5.627	-15.775	1.00	1.03
ATOM	1840	C	LEU	125	-8.256	-8.044	-11.234	1.00	0.24
ATOM	1841	O	LEU	125	-8.790	-8.935	-11.864	1.00	0.33
ATOM	1842	N	GLY	126	-8.277	-8.035	-9.927	1.00	0.24
ATOM	1843	HN	GLY	126	-7.858	-7.298	-9.435	1.00	0.29
ATOM	1844	CA	GLY	126	-8.968	-9.132	-9.185	1.00	0.27
ATOM	1845	HA1	GLY	126	-9.748	-9.545	-9.807	1.00	0.29
ATOM	1846	HA2	GLY	126	-9.408	-8.727	-8.285	1.00	0.29
ATOM	1847	C	GLY	126	-7.985	-10.245	-8.809	1.00	0.26
ATOM	1848	O	GLY	126	-8.377	-11.268	-8.283	1.00	0.30
ATOM	1849	N	LEU	127	-6.719	-10.068	-9.063	1.00	0.23
ATOM	1850	HN	LEU	127	-6.410	-9.239	-9.484	1.00	0.22
ATOM	1851	CA	LEU	127	-5.744	-11.138	-8.700	1.00	0.25
ATOM	1852	HA	LEU	127	-6.212	-12.099	-8.815	1.00	0.28
ATOM	1853	CB	LEU	127	-4.507	-11.052	-9.602	1.00	0.23
ATOM	1854	HB1	LEU	127	-3.733	-11.696	-9.211	1.00	0.25
ATOM	1855	HB2	LEU	127	-4.156	-10.033	-9.602	1.00	0.22
ATOM	1856	CG	LEU	127	-4.844	-11.471	-11.045	1.00	0.24
ATOM	1857	HG	LEU	127	-5.707	-10.915	-11.384	1.00	0.23
ATOM	1858	CD1	LEU	127	-3.646	-11.159	-11.962	1.00	0.24
ATOM	1859	HD11	LEU	127	-4.001	-10.692	-12.868	1.00	1.00
ATOM	1860	HD12	LEU	127	-3.126	-12.073	-12.208	1.00	1.02
ATOM	1861	HD13	LEU	127	-2.962	-10.491	-11.460	1.00	1.03
ATOM	1862	CD2	LEU	127	-5.150	-12.980	-11.109	1.00	0.30
ATOM	1863	HD21	LEU	127	-5.021	-13.334	-12.121	1.00	1.04
ATOM	1864	HD22	LEU	127	-6.169	-13.159	-10.805	1.00	1.11
ATOM	1865	HD23	LEU	127	-4.478	-13.515	-10.454	1.00	1.03
ATOM	1866	C	LEU	127	-5.315	-10.969	-7.241	1.00	0.28
ATOM	1867	O	LEU	127	-5.245	-9.872	-6.723	1.00	0.32
ATOM	1868	N	ASP	128	-5.027	-12.059	-6.581	1.00	0.32
ATOM	1869	HN	ASP	128	-5.093	-12.928	-7.029	1.00	0.34
ATOM	1870	CA	ASP	128	-4.598	-11.997	-5.154	1.00	0.39
ATOM	1871	HA	ASP	128	-4.882	-11.046	-4.728	1.00	0.40
ATOM	1872	CB	ASP	128	-5.271	-13.130	-4.375	1.00	0.48
ATOM	1873	HB1	ASP	128	-4.779	-14.064	-4.600	1.00	0.48
ATOM	1874	HB2	ASP	128	-6.311	-13.193	-4.661	1.00	0.50
ATOM	1875	CG	ASP	128	-5.171	-12.854	-2.873	1.00	0.55
ATOM	1876	OD1	ASP	128	-4.082	-12.980	-2.339	1.00	1.23
ATOM	1877	OD2	ASP	128	-6.185	-12.521	-2.283	1.00	1.22
ATOM	1878	C	ASP	128	-3.078	-12.159	-5.082	1.00	0.37
ATOM	1879	O	ASP	128	-2.424	-12.387	-6.080	1.00	0.59
ATOM	1880	N	HIS	129	-2.507	-12.042	-3.914	1.00	0.23
ATOM	1881	HN	HIS	129	-3.048	-11.856	-3.118	1.00	0.32
ATOM	1882	CA	HIS	129	-1.029	-12.189	-3.797	1.00	0.22
ATOM	1883	HA	HIS	129	-0.543	-11.439	-4.401	1.00	0.21
ATOM	1884	CB	HIS	129	-0.606	-12.019	-2.335	1.00	0.23
ATOM	1885	HB1	HIS	129	0.430	-12.302	-2.227	1.00	0.24
ATOM	1886	HB2	HIS	129	-1.217	-12.653	-1.710	1.00	0.25
ATOM	1887	CG	HIS	129	-0.779	-10.585	-1.912	1.00	0.22

ATOM	1888	ND1	HIS	129	-1.862	-10.161	-1.156	1.00	0.35
ATOM	1889	HD1	HIS	129	-2.602	-10.720	-0.841	1.00	0.53
ATOM	1890	CD2	HIS	129	-0.007	-9.468	-2.118	1.00	0.34
ATOM	1891	HD2	HIS	129	0.918	-9.447	-2.673	1.00	0.54
ATOM	1892	CE1	HIS	129	-1.711	-8.842	-0.936	1.00	0.31
ATOM	1893	HE1	HIS	129	-2.406	-8.239	-0.370	1.00	0.44
ATOM	1894	NE2	HIS	129	-0.597	-8.369	-1.501	1.00	0.28
ATOM	1895	C	HIS	129	-0.614	-13.584	-4.277	1.00	0.24
ATOM	1896	O	HIS	129	-1.267	-14.568	-3.991	1.00	0.28
ATOM	1897	N	SER	130	0.474	-13.671	-4.999	1.00	0.24
ATOM	1898	HN	SER	130	0.984	-12.862	-5.210	1.00	0.23
ATOM	1899	CA	SER	130	0.949	-14.996	-5.498	1.00	0.29
ATOM	1900	HA	SER	130	0.139	-15.710	-5.464	1.00	0.33
ATOM	1901	CB	SER	130	1.442	-14.852	-6.938	1.00	0.32
ATOM	1902	HB1	SER	130	2.201	-14.082	-6.982	1.00	0.31
ATOM	1903	HB2	SER	130	0.618	-14.577	-7.576	1.00	0.35
ATOM	1904	OG	SER	130	1.980	-16.092	-7.378	1.00	0.40
ATOM	1905	HG	SER	130	1.254	-16.714	-7.469	1.00	0.97
ATOM	1906	C	SER	130	2.096	-15.484	-4.609	1.00	0.28
ATOM	1907	O	SER	130	2.801	-14.696	-4.009	1.00	0.29
ATOM	1908	N	LYS	131	2.287	-16.775	-4.514	1.00	0.30
ATOM	1909	HN	LYS	131	1.705	-17.393	-5.003	1.00	0.32
ATOM	1910	CA	LYS	131	3.386	-17.310	-3.656	1.00	0.32
ATOM	1911	HA	LYS	131	3.665	-16.567	-2.923	1.00	0.34
ATOM	1912	CB	LYS	131	2.903	-18.572	-2.936	1.00	0.39
ATOM	1913	HB1	LYS	131	3.714	-18.988	-2.355	1.00	0.42
ATOM	1914	HB2	LYS	131	2.572	-19.298	-3.664	1.00	0.40
ATOM	1915	CG	LYS	131	1.743	-18.214	-2.003	1.00	0.45
ATOM	1916	HG1	LYS	131	0.932	-17.798	-2.581	1.00	0.79
ATOM	1917	HG2	LYS	131	2.077	-17.488	-1.276	1.00	1.01
ATOM	1918	CD	LYS	131	1.255	-19.472	-1.280	1.00	1.18
ATOM	1919	HD1	LYS	131	2.064	-19.890	-0.698	1.00	1.86
ATOM	1920	HD2	LYS	131	0.921	-20.199	-2.006	1.00	1.66
ATOM	1921	CE	LYS	131	0.096	-19.108	-0.349	1.00	1.52
ATOM	1922	HE1	LYS	131	-0.788	-18.908	-0.937	1.00	1.92
ATOM	1923	HE2	LYS	131	0.355	-18.229	0.222	1.00	1.93
ATOM	1924	NZ	LYS	131	-0.174	-20.242	0.581	1.00	2.23
ATOM	1925	HZ1	LYS	131	-1.103	-20.109	1.030	1.00	2.72
ATOM	1926	HZ2	LYS	131	0.565	-20.272	1.313	1.00	2.53
ATOM	1927	HZ3	LYS	131	-0.174	-21.135	0.050	1.00	2.72
ATOM	1928	C	LYS	131	4.604	-17.649	-4.521	1.00	0.31
ATOM	1929	O	LYS	131	5.612	-18.116	-4.027	1.00	0.34
ATOM	1930	N	ASP	132	4.532	-17.411	-5.804	1.00	0.29
ATOM	1931	HN	ASP	132	3.717	-17.028	-6.190	1.00	0.28
ATOM	1932	CA	ASP	132	5.703	-17.719	-6.674	1.00	0.30
ATOM	1933	HA	ASP	132	6.187	-18.601	-6.302	1.00	0.32
ATOM	1934	CB	ASP	132	5.225	-17.970	-8.108	1.00	0.32
ATOM	1935	HB1	ASP	132	4.727	-17.090	-8.483	1.00	0.31
ATOM	1936	HB2	ASP	132	4.539	-18.804	-8.118	1.00	0.34
ATOM	1937	CG	ASP	132	6.430	-18.289	-8.996	1.00	0.35
ATOM	1938	OD1	ASP	132	6.457	-19.371	-9.558	1.00	1.10
ATOM	1939	OD2	ASP	132	7.306	-17.446	-9.097	1.00	1.15
ATOM	1940	C	ASP	132	6.656	-16.501	-6.659	1.00	0.28
ATOM	1941	O	ASP	132	6.226	-15.399	-6.939	1.00	0.28
ATOM	1942	N	PRO	133	7.930	-16.658	-6.328	1.00	0.30
ATOM	1943	CA	PRO	133	8.852	-15.484	-6.296	1.00	0.31
ATOM	1944	HA	PRO	133	8.517	-14.766	-5.566	1.00	0.32
ATOM	1945	CB	PRO	133	10.173	-16.097	-5.832	1.00	0.36
ATOM	1946	HB1	PRO	133	10.441	-15.694	-4.867	1.00	0.36
ATOM	1947	HB2	PRO	133	10.949	-15.869	-6.549	1.00	0.41
ATOM	1948	CG	PRO	133	10.007	-17.615	-5.721	1.00	0.42
ATOM	1949	HG1	PRO	133	10.293	-17.940	-4.732	1.00	0.51
ATOM	1950	HG2	PRO	133	10.630	-18.103	-6.457	1.00	0.51
ATOM	1951	CD	PRO	133	8.540	-17.972	-5.969	1.00	0.35
ATOM	1952	HD2	PRO	133	8.456	-18.679	-6.785	1.00	0.34
ATOM	1953	HD1	PRO	133	8.091	-18.362	-5.069	1.00	0.38
ATOM	1954	C	PRO	133	9.032	-14.810	-7.662	1.00	0.31
ATOM	1955	O	PRO	133	9.496	-13.691	-7.749	1.00	0.34
ATOM	1956	N	GLY	134	8.684	-15.477	-8.729	1.00	0.32
ATOM	1957	HN	GLY	134	8.320	-16.382	-8.647	1.00	0.35
ATOM	1958	CA	GLY	134	8.860	-14.856	-10.074	1.00	0.34
ATOM	1959	HA1	GLY	134	9.048	-15.630	-10.803	1.00	0.37
ATOM	1960	HA2	GLY	134	9.701	-14.177	-10.047	1.00	0.36
ATOM	1961	C	GLY	134	7.598	-14.087	-10.471	1.00	0.29
ATOM	1962	O	GLY	134	7.563	-13.420	-11.486	1.00	0.29
ATOM	1963	N	ALA	135	6.563	-14.168	-9.683	1.00	0.27
ATOM	1964	HN	ALA	135	6.607	-14.709	-8.867	1.00	0.28

ATOM	1965	CA	ALA	135	5.312	-13.434	-10.026	1.00	0.24
ATOM	1966	HA	ALA	135	5.199	-13.401	-11.099	1.00	0.25
ATOM	1967	CB	ALA	135	4.109	-14.151	-9.410	1.00	0.25
ATOM	1968	HB1	ALA	135	3.633	-14.765	-10.160	1.00	1.07
ATOM	1969	HB2	ALA	135	3.405	-13.421	-9.041	1.00	1.01
ATOM	1970	HB3	ALA	135	4.442	-14.774	-8.593	1.00	1.04
ATOM	1971	C	ALA	135	5.388	-12.007	-9.479	1.00	0.21
ATOM	1972	O	ALA	135	5.968	-11.760	-8.440	1.00	0.23
ATOM	1973	N	LEU	136	4.799	-11.067	-10.164	1.00	0.22
ATOM	1974	HN	LEU	136	4.330	-11.286	-10.996	1.00	0.24
ATOM	1975	CA	LEU	136	4.830	-9.660	-9.676	1.00	0.23
ATOM	1976	HA	LEU	136	5.842	-9.382	-9.427	1.00	0.25
ATOM	1977	CB	LEU	136	4.279	-8.724	-10.761	1.00	0.25
ATOM	1978	HB1	LEU	136	4.193	-7.724	-10.365	1.00	0.27
ATOM	1979	HB2	LEU	136	3.302	-9.072	-11.064	1.00	0.26
ATOM	1980	CG	LEU	136	5.213	-8.709	-11.980	1.00	0.26
ATOM	1981	HG	LEU	136	5.312	-9.713	-12.368	1.00	0.29
ATOM	1982	CD1	LEU	136	4.624	-7.801	-13.063	1.00	0.29
ATOM	1983	HD11	LEU	136	3.546	-7.848	-13.030	1.00	1.06
ATOM	1984	HD12	LEU	136	4.967	-8.126	-14.033	1.00	1.05
ATOM	1985	HD13	LEU	136	4.944	-6.784	-12.893	1.00	1.06
ATOM	1986	CD2	LEU	136	6.592	-8.176	-11.578	1.00	0.32
ATOM	1987	HD21	LEU	136	6.485	-7.477	-10.762	1.00	1.05
ATOM	1988	HD22	LEU	136	7.046	-7.677	-12.422	1.00	1.09
ATOM	1989	HD23	LEU	136	7.220	-8.998	-11.269	1.00	0.97
ATOM	1990	C	LEU	136	3.954	-9.556	-8.427	1.00	0.25
ATOM	1991	O	LEU	136	4.201	-8.761	-7.542	1.00	0.30
ATOM	1992	N	MET	137	2.924	-10.353	-8.357	1.00	0.28
ATOM	1993	HN	MET	137	2.744	-10.981	-9.087	1.00	0.31
ATOM	1994	CA	MET	137	2.016	-10.309	-7.177	1.00	0.33
ATOM	1995	HA	MET	137	1.768	-9.283	-6.959	1.00	0.38
ATOM	1996	CB	MET	137	0.734	-11.087	-7.494	1.00	0.42
ATOM	1997	HB1	MET	137	0.118	-11.136	-6.615	1.00	0.57
ATOM	1998	HB2	MET	137	0.995	-12.089	-7.803	1.00	0.50
ATOM	1999	CG	MET	137	-0.035	-10.391	-8.625	1.00	0.58
ATOM	2000	HG1	MET	137	-0.909	-10.975	-8.875	1.00	1.13
ATOM	2001	HG2	MET	137	0.601	-10.311	-9.494	1.00	1.22
ATOM	2002	SD	MET	137	-0.551	-8.729	-8.108	1.00	0.83
ATOM	2003	CE	MET	137	-2.048	-9.184	-7.194	1.00	0.39
ATOM	2004	HE1	MET	137	-2.231	-8.450	-6.426	1.00	1.14
ATOM	2005	HE2	MET	137	-1.927	-10.151	-6.741	1.00	1.07
ATOM	2006	HE3	MET	137	-2.885	-9.212	-7.872	1.00	1.06
ATOM	2007	C	MET	137	2.700	-10.925	-5.951	1.00	0.27
ATOM	2008	O	MET	137	2.050	-11.287	-4.990	1.00	0.28
ATOM	2009	N	PHE	138	4.000	-11.042	-5.964	1.00	0.25
ATOM	2010	HN	PHE	138	4.514	-10.741	-6.743	1.00	0.28
ATOM	2011	CA	PHE	138	4.699	-11.628	-4.785	1.00	0.23
ATOM	2012	HA	PHE	138	4.225	-12.557	-4.534	1.00	0.26
ATOM	2013	CB	PHE	138	6.167	-11.877	-5.152	1.00	0.25
ATOM	2014	HB1	PHE	138	6.710	-10.945	-5.104	1.00	0.24
ATOM	2015	HB2	PHE	138	6.221	-12.270	-6.156	1.00	0.27
ATOM	2016	CG	PHE	138	6.790	-12.873	-4.194	1.00	0.28
ATOM	2017	CD1	PHE	138	6.295	-14.184	-4.113	1.00	0.32
ATOM	2018	HD1	PHE	138	5.465	-14.490	-4.731	1.00	0.33
ATOM	2019	CD2	PHE	138	7.871	-12.486	-3.392	1.00	0.30
ATOM	2020	HD2	PHE	138	8.256	-11.481	-3.455	1.00	0.30
ATOM	2021	CE1	PHE	138	6.881	-15.100	-3.230	1.00	0.38
ATOM	2022	HE1	PHE	138	6.500	-16.109	-3.168	1.00	0.42
ATOM	2023	CE2	PHE	138	8.455	-13.404	-2.511	1.00	0.36
ATOM	2024	HE2	PHE	138	9.288	-13.104	-1.894	1.00	0.39
ATOM	2025	CZ	PHE	138	7.960	-14.710	-2.430	1.00	0.39
ATOM	2026	HZ	PHE	138	8.411	-15.417	-1.749	1.00	0.44
ATOM	2027	C	PHE	138	4.601	-10.615	-3.615	1.00	0.20
ATOM	2028	O	PHE	138	4.874	-9.447	-3.808	1.00	0.22
ATOM	2029	N	PRO	139	4.185	-11.019	-2.421	1.00	0.22
ATOM	2030	CA	PRO	139	4.044	-10.048	-1.291	1.00	0.25
ATOM	2031	HA	PRO	139	3.262	-9.340	-1.509	1.00	0.27
ATOM	2032	CB	PRO	139	3.600	-10.936	-0.127	1.00	0.31
ATOM	2033	HB1	PRO	139	2.615	-10.638	0.199	1.00	0.38
ATOM	2034	HB2	PRO	139	4.299	-10.835	0.691	1.00	0.42
ATOM	2035	CG	PRO	139	3.562	-12.392	-0.597	1.00	0.33
ATOM	2036	HG1	PRO	139	2.588	-12.812	-0.396	1.00	0.41
ATOM	2037	HG2	PRO	139	4.317	-12.961	-0.074	1.00	0.42
ATOM	2038	CD	PRO	139	3.834	-12.435	-2.102	1.00	0.27
ATOM	2039	HD2	PRO	139	4.661	-13.100	-2.318	1.00	0.28
ATOM	2040	HD1	PRO	139	2.946	-12.732	-2.637	1.00	0.30
ATOM	2041	C	PRO	139	5.337	-9.305	-0.926	1.00	0.26

ATOM	2042	O	PRO	139	5.302	-8.351	-0.173	1.00	0.44
ATOM	2043	N	ILE	140	6.467	-9.726	-1.437	1.00	0.24
ATOM	2044	HN	ILE	140	6.474	-10.500	-2.038	1.00	0.37
ATOM	2045	CA	ILE	140	7.749	-9.031	-1.094	1.00	0.23
ATOM	2046	HA	ILE	140	7.572	-8.308	-0.312	1.00	0.24
ATOM	2047	CB	ILE	140	8.775	-10.054	-0.600	1.00	0.25
ATOM	2048	HB	ILE	140	8.978	-10.770	-1.379	1.00	0.25
ATOM	2049	CG1	ILE	140	8.207	-10.768	0.632	1.00	0.29
ATOM	2050	HG11	ILE	140	7.246	-11.196	0.384	1.00	0.32
ATOM	2051	HG12	ILE	140	8.084	-10.055	1.434	1.00	0.33
ATOM	2052	CG2	ILE	140	10.070	-9.332	-0.214	1.00	0.26
ATOM	2053	HG21	ILE	140	9.850	-8.567	0.517	1.00	1.04
ATOM	2054	HG22	ILE	140	10.505	-8.876	-1.090	1.00	1.06
ATOM	2055	HG23	ILE	140	10.768	-10.040	0.207	1.00	1.04
ATOM	2056	CD1	ILE	140	9.156	-11.883	1.082	1.00	0.30
ATOM	2057	HD11	ILE	140	9.716	-12.250	0.236	1.00	1.08
ATOM	2058	HD12	ILE	140	8.582	-12.691	1.511	1.00	0.98
ATOM	2059	HD13	ILE	140	9.838	-11.495	1.824	1.00	1.08
ATOM	2060	C	ILE	140	8.284	-8.301	-2.329	1.00	0.22
ATOM	2061	O	ILE	140	8.265	-8.817	-3.429	1.00	0.22
ATOM	2062	N	TYR	141	8.745	-7.092	-2.150	1.00	0.21
ATOM	2063	HN	TYR	141	8.736	-6.696	-1.254	1.00	0.22
ATOM	2064	CA	TYR	141	9.265	-6.303	-3.304	1.00	0.21
ATOM	2065	HA	TYR	141	8.560	-6.348	-4.120	1.00	0.20
ATOM	2066	CB	TYR	141	9.444	-4.847	-2.865	1.00	0.21
ATOM	2067	HB1	TYR	141	10.050	-4.810	-1.972	1.00	0.22
ATOM	2068	HB2	TYR	141	8.476	-4.413	-2.661	1.00	0.22
ATOM	2069	CG	TYR	141	10.122	-4.066	-3.962	1.00	0.23
ATOM	2070	CD1	TYR	141	11.515	-4.104	-4.089	1.00	0.25
ATOM	2071	HD1	TYR	141	12.104	-4.697	-3.404	1.00	0.26
ATOM	2072	CD2	TYR	141	9.359	-3.298	-4.848	1.00	0.24
ATOM	2073	HD2	TYR	141	8.284	-3.268	-4.750	1.00	0.25
ATOM	2074	CE1	TYR	141	12.146	-3.376	-5.103	1.00	0.28
ATOM	2075	HE1	TYR	141	13.221	-3.405	-5.201	1.00	0.32
ATOM	2076	CE2	TYR	141	9.989	-2.569	-5.862	1.00	0.27
ATOM	2077	HE2	TYR	141	9.401	-1.975	-6.544	1.00	0.30
ATOM	2078	CZ	TYR	141	11.383	-2.608	-5.990	1.00	0.29
ATOM	2079	OH	TYR	141	12.005	-1.892	-6.991	1.00	0.33
ATOM	2080	HH	TYR	141	12.781	-2.385	-7.269	1.00	0.90
ATOM	2081	C	TYR	141	10.615	-6.864	-3.761	1.00	0.22
ATOM	2082	O	TYR	141	11.522	-7.050	-2.973	1.00	0.23
ATOM	2083	N	THR	142	10.750	-7.130	-5.035	1.00	0.22
ATOM	2084	HN	THR	142	10.002	-6.968	-5.648	1.00	0.22
ATOM	2085	CA	THR	142	12.035	-7.675	-5.563	1.00	0.24
ATOM	2086	HA	THR	142	12.835	-7.447	-4.874	1.00	0.25
ATOM	2087	CB	THR	142	11.917	-9.193	-5.723	1.00	0.25
ATOM	2088	HB	THR	142	11.645	-9.635	-4.777	1.00	0.26
ATOM	2089	OG1	THR	142	13.165	-9.720	-6.152	1.00	0.29
ATOM	2090	HG1	THR	142	13.274	-9.505	-7.081	1.00	0.97
ATOM	2091	CG2	THR	142	10.840	-9.517	-6.760	1.00	0.25
ATOM	2092	HG21	THR	142	10.577	-10.562	-6.691	1.00	1.04
ATOM	2093	HG22	THR	142	11.217	-9.304	-7.749	1.00	1.05
ATOM	2094	HG23	THR	142	9.965	-8.913	-6.570	1.00	1.06
ATOM	2095	C	THR	142	12.339	-7.040	-6.924	1.00	0.23
ATOM	2096	O	THR	142	11.454	-6.810	-7.724	1.00	0.23
ATOM	2097	N	TYR	143	13.586	-6.758	-7.195	1.00	0.25
ATOM	2098	HN	TYR	143	14.285	-6.955	-6.538	1.00	0.27
ATOM	2099	CA	TYR	143	13.948	-6.144	-8.506	1.00	0.26
ATOM	2100	HA	TYR	143	13.174	-5.452	-8.804	1.00	0.25
ATOM	2101	CB	TYR	143	15.277	-5.395	-8.370	1.00	0.29
ATOM	2102	HB1	TYR	143	16.072	-6.104	-8.190	1.00	0.33
ATOM	2103	HB2	TYR	143	15.217	-4.704	-7.542	1.00	0.30
ATOM	2104	CG	TYR	143	15.563	-4.633	-9.642	1.00	0.27
ATOM	2105	CD1	TYR	143	14.931	-3.406	-9.880	1.00	0.25
ATOM	2106	HD1	TYR	143	14.234	-3.008	-9.156	1.00	0.26
ATOM	2107	CD2	TYR	143	16.466	-5.148	-10.581	1.00	0.31
ATOM	2108	HD2	TYR	143	16.954	-6.094	-10.398	1.00	0.35
ATOM	2109	CE1	TYR	143	15.201	-2.695	-11.055	1.00	0.26
ATOM	2110	HE1	TYR	143	14.713	-1.749	-11.238	1.00	0.28
ATOM	2111	CE2	TYR	143	16.735	-4.436	-11.756	1.00	0.31
ATOM	2112	HE2	TYR	143	17.432	-4.833	-12.480	1.00	0.36
ATOM	2113	CZ	TYR	143	16.103	-3.210	-11.994	1.00	0.28
ATOM	2114	OH	TYR	143	16.369	-2.509	-13.152	1.00	0.30
ATOM	2115	HH	TYR	143	17.068	-2.969	-13.624	1.00	0.95
ATOM	2116	C	TYR	143	14.080	-7.244	-9.563	1.00	0.27
ATOM	2117	O	TYR	143	14.552	-8.328	-9.283	1.00	0.31
ATOM	2118	N	THR	144	13.660	-6.876	-10.772	1.00	0.29

ATOM	2119	HN	THR	144	13.277	-6.096	-10.972	1.00	0.32
ATOM	2120	CA	THR	144	13.753	-8.008	-11.847	1.00	0.32
ATOM	2121	HA	THR	144	14.479	-8.758	-11.573	1.00	0.35
ATOM	2122	CB	THR	144	12.385	-8.666	-12.031	1.00	0.37
ATOM	2123	HB	THR	144	11.922	-8.814	-11.067	1.00	0.84
ATOM	2124	OG1	THR	144	12.549	-9.918	-12.683	1.00	1.00
ATOM	2125	HG1	THR	144	13.280	-9.836	-13.301	1.00	1.42
ATOM	2126	CG2	THR	144	11.499	-7.757	-12.882	1.00	0.82
ATOM	2127	HG21	THR	144	10.461	-7.991	-12.699	1.00	1.51
ATOM	2128	HG22	THR	144	11.724	-7.911	-13.927	1.00	1.24
ATOM	2129	HG23	THR	144	11.687	-6.726	-12.622	1.00	1.49
ATOM	2130	C	THR	144	14.169	-7.351	-13.165	1.00	0.34
ATOM	2131	O	THR	144	13.922	-6.183	-13.392	1.00	0.32
ATOM	2132	N	GLY	145	14.789	-8.094	-14.043	1.00	0.43
ATOM	2133	HN	GLY	145	14.971	-9.037	-13.846	1.00	0.49
ATOM	2134	CA	GLY	145	15.205	-7.510	-15.350	1.00	0.49
ATOM	2135	HA1	GLY	145	15.842	-8.207	-15.872	1.00	0.57
ATOM	2136	HA2	GLY	145	15.742	-6.587	-15.178	1.00	0.50
ATOM	2137	C	GLY	145	13.957	-7.233	-16.191	1.00	0.47
ATOM	2138	O	GLY	145	13.331	-8.138	-16.706	1.00	0.53
ATOM	2139	N	LYS	146	13.583	-5.990	-16.322	1.00	0.46
ATOM	2140	HN	LYS	146	14.097	-5.277	-15.889	1.00	0.48
ATOM	2141	CA	LYS	146	12.367	-5.653	-17.116	1.00	0.49
ATOM	2142	HA	LYS	146	11.578	-6.350	-16.876	1.00	0.51
ATOM	2143	CB	LYS	146	11.911	-4.235	-16.764	1.00	0.52
ATOM	2144	HB1	LYS	146	10.973	-4.032	-17.254	1.00	0.58
ATOM	2145	HB2	LYS	146	12.657	-3.533	-17.103	1.00	0.57
ATOM	2146	CG	LYS	146	11.744	-4.128	-15.238	1.00	0.55
ATOM	2147	HG1	LYS	146	12.690	-3.853	-14.798	1.00	0.83
ATOM	2148	HG2	LYS	146	11.442	-5.089	-14.849	1.00	1.14
ATOM	2149	CD	LYS	146	10.684	-3.077	-14.854	1.00	1.23
ATOM	2150	HD1	LYS	146	10.308	-3.309	-13.871	1.00	1.78
ATOM	2151	HD2	LYS	146	9.865	-3.098	-15.556	1.00	1.79
ATOM	2152	CE	LYS	146	11.298	-1.671	-14.828	1.00	2.01
ATOM	2153	HE1	LYS	146	11.615	-1.439	-13.822	1.00	2.47
ATOM	2154	HE2	LYS	146	10.556	-0.952	-15.143	1.00	2.39
ATOM	2155	NZ	LYS	146	12.468	-1.601	-15.745	1.00	2.91
ATOM	2156	HZ1	LYS	146	12.847	-0.633	-15.750	1.00	3.39
ATOM	2157	HZ2	LYS	146	12.170	-1.861	-16.707	1.00	3.28
ATOM	2158	HZ3	LYS	146	13.205	-2.257	-15.420	1.00	3.27
ATOM	2159	C	LYS	146	12.677	-5.732	-18.613	1.00	0.59
ATOM	2160	O	LYS	146	11.845	-5.426	-19.444	1.00	1.16
ATOM	2161	N	SER	147	13.868	-6.131	-18.967	1.00	0.78
ATOM	2162	HN	SER	147	14.530	-6.366	-18.283	1.00	1.26
ATOM	2163	CA	SER	147	14.226	-6.214	-20.413	1.00	0.87
ATOM	2164	HA	SER	147	14.141	-5.234	-20.859	1.00	1.03
ATOM	2165	CB	SER	147	15.667	-6.709	-20.554	1.00	0.95
ATOM	2166	HB1	SER	147	15.798	-7.158	-21.530	1.00	1.42
ATOM	2167	HB2	SER	147	15.871	-7.445	-19.794	1.00	1.34
ATOM	2168	OG	SER	147	16.561	-5.616	-20.395	1.00	1.71
ATOM	2169	HG	SER	147	17.097	-5.555	-21.190	1.00	2.16
ATOM	2170	C	SER	147	13.288	-7.185	-21.138	1.00	0.79
ATOM	2171	O	SER	147	12.747	-6.865	-22.178	1.00	1.40
ATOM	2172	N	HIS	148	13.098	-8.366	-20.605	1.00	0.66
ATOM	2173	HN	HIS	148	13.551	-8.602	-19.768	1.00	1.10
ATOM	2174	CA	HIS	148	12.199	-9.360	-21.272	1.00	0.65
ATOM	2175	HA	HIS	148	11.629	-8.874	-22.048	1.00	0.74
ATOM	2176	CB	HIS	148	13.041	-10.479	-21.887	1.00	0.79
ATOM	2177	HB1	HIS	148	12.401	-11.312	-22.138	1.00	1.14
ATOM	2178	HB2	HIS	148	13.786	-10.801	-21.174	1.00	1.30
ATOM	2179	CG	HIS	148	13.723	-9.980	-23.130	1.00	1.66
ATOM	2180	ND1	HIS	148	13.104	-9.116	-24.019	1.00	2.52
ATOM	2181	HD1	HIS	148	12.200	-8.747	-23.934	1.00	2.81
ATOM	2182	CD2	HIS	148	14.969	-10.226	-23.652	1.00	2.62
ATOM	2183	HD2	HIS	148	15.715	-10.867	-23.206	1.00	3.00
ATOM	2184	CE1	HIS	148	13.970	-8.875	-25.020	1.00	3.46
ATOM	2185	HE1	HIS	148	13.759	-8.233	-25.863	1.00	4.33
ATOM	2186	NE2	HIS	148	15.123	-9.528	-24.846	1.00	3.55
ATOM	2187	C	HIS	148	11.238	-9.971	-20.249	1.00	0.55
ATOM	2188	O	HIS	148	10.743	-11.064	-20.435	1.00	0.60
ATOM	2189	N	PHE	149	10.978	-9.293	-19.167	1.00	0.57
ATOM	2190	HN	PHE	149	11.392	-8.417	-19.021	1.00	0.73
ATOM	2191	CA	PHE	149	10.060	-9.871	-18.145	1.00	0.48
ATOM	2192	HA	PHE	149	10.416	-10.849	-17.857	1.00	0.51
ATOM	2193	CB	PHE	149	10.022	-8.967	-16.911	1.00	0.44
ATOM	2194	HB1	PHE	149	9.603	-8.008	-17.177	1.00	0.44
ATOM	2195	HB2	PHE	149	11.023	-8.831	-16.530	1.00	0.48

ATOM	2196	CG	PHE	149	9.161	-9.615	-15.851	1.00	0.40
ATOM	2197	CD1	PHE	149	7.766	-9.507	-15.919	1.00	0.36
ATOM	2198	HD1	PHE	149	7.305	-8.956	-16.726	1.00	0.38
ATOM	2199	CD2	PHE	149	9.757	-10.328	-14.804	1.00	0.42
ATOM	2200	HD2	PHE	149	10.832	-10.412	-14.750	1.00	0.48
ATOM	2201	CE1	PHE	149	6.969	-10.112	-14.941	1.00	0.35
ATOM	2202	HE1	PHE	149	5.894	-10.031	-14.996	1.00	0.37
ATOM	2203	CE2	PHE	149	8.958	-10.932	-13.825	1.00	0.40
ATOM	2204	HE2	PHE	149	9.417	-11.482	-13.016	1.00	0.45
ATOM	2205	CZ	PHE	149	7.564	-10.825	-13.894	1.00	0.37
ATOM	2206	HZ	PHE	149	6.948	-11.291	-13.140	1.00	0.38
ATOM	2207	C	PHE	149	8.641	-9.993	-18.706	1.00	0.43
ATOM	2208	O	PHE	149	8.080	-9.044	-19.217	1.00	0.45
ATOM	2209	N	MET	150	8.050	-11.153	-18.575	1.00	0.43
ATOM	2210	HN	MET	150	8.523	-11.888	-18.133	1.00	0.50
ATOM	2211	CA	MET	150	6.651	-11.357	-19.051	1.00	0.39
ATOM	2212	HA	MET	150	6.189	-10.400	-19.245	1.00	0.38
ATOM	2213	CB	MET	150	6.632	-12.207	-20.328	1.00	0.44
ATOM	2214	HB1	MET	150	5.610	-12.374	-20.632	1.00	0.45
ATOM	2215	HB2	MET	150	7.109	-13.157	-20.134	1.00	0.47
ATOM	2216	CG	MET	150	7.381	-11.477	-21.446	1.00	0.50
ATOM	2217	HG1	MET	150	8.401	-11.831	-21.485	1.00	0.98
ATOM	2218	HG2	MET	150	7.376	-10.415	-21.253	1.00	0.86
ATOM	2219	SD	MET	150	6.571	-11.806	-23.033	1.00	1.32
ATOM	2220	CE	MET	150	7.378	-13.384	-23.393	1.00	2.23
ATOM	2221	HE1	MET	150	7.326	-14.022	-22.521	1.00	2.66
ATOM	2222	HE2	MET	150	8.411	-13.211	-23.647	1.00	2.74
ATOM	2223	HE3	MET	150	6.879	-13.861	-24.225	1.00	2.74
ATOM	2224	C	MET	150	5.877	-12.071	-17.943	1.00	0.32
ATOM	2225	O	MET	150	6.435	-12.837	-17.183	1.00	0.32
ATOM	2226	N	LEU	151	4.605	-11.819	-17.827	1.00	0.28
ATOM	2227	HN	LEU	151	4.169	-11.188	-18.437	1.00	0.30
ATOM	2228	CA	LEU	151	3.821	-12.478	-16.746	1.00	0.24
ATOM	2229	HA	LEU	151	4.120	-12.064	-15.803	1.00	0.24
ATOM	2230	CB	LEU	151	2.327	-12.212	-16.966	1.00	0.24
ATOM	2231	HB1	LEU	151	1.765	-12.626	-16.145	1.00	0.25
ATOM	2232	HB2	LEU	151	2.012	-12.680	-17.887	1.00	0.28
ATOM	2233	CG	LEU	151	2.061	-10.703	-17.047	1.00	0.28
ATOM	2234	HG	LEU	151	2.900	-10.208	-17.512	1.00	0.52
ATOM	2235	CD1	LEU	151	0.804	-10.457	-17.881	1.00	0.35
ATOM	2236	HD11	LEU	151	0.506	-9.424	-17.788	1.00	1.07
ATOM	2237	HD12	LEU	151	0.007	-11.095	-17.526	1.00	1.02
ATOM	2238	HD13	LEU	151	1.009	-10.682	-18.917	1.00	1.17
ATOM	2239	CD2	LEU	151	1.848	-10.140	-15.638	1.00	0.46
ATOM	2240	HD21	LEU	151	2.078	-9.084	-15.635	1.00	1.14
ATOM	2241	HD22	LEU	151	2.495	-10.650	-14.941	1.00	1.16
ATOM	2242	HD23	LEU	151	0.820	-10.284	-15.345	1.00	1.11
ATOM	2243	C	LEU	151	4.076	-14.004	-16.794	1.00	0.24
ATOM	2244	O	LEU	151	3.879	-14.613	-17.826	1.00	0.28
ATOM	2245	N	PRO	152	4.504	-14.641	-15.711	1.00	0.22
ATOM	2246	CA	PRO	152	4.748	-16.112	-15.751	1.00	0.23
ATOM	2247	HA	PRO	152	5.480	-16.354	-16.503	1.00	0.24
ATOM	2248	CB	PRO	152	5.323	-16.404	-14.364	1.00	0.24
ATOM	2249	HB1	PRO	152	6.361	-16.686	-14.453	1.00	0.29
ATOM	2250	HB2	PRO	152	4.766	-17.208	-13.903	1.00	0.26
ATOM	2251	CG	PRO	152	5.209	-15.141	-13.507	1.00	0.32
ATOM	2252	HG1	PRO	152	6.166	-14.917	-13.061	1.00	0.44
ATOM	2253	HG2	PRO	152	4.473	-15.295	-12.730	1.00	0.41
ATOM	2254	CD	PRO	152	4.778	-13.976	-14.402	1.00	0.25
ATOM	2255	HD2	PRO	152	3.886	-13.507	-14.008	1.00	0.25
ATOM	2256	HD1	PRO	152	5.581	-13.263	-14.503	1.00	0.27
ATOM	2257	C	PRO	152	3.462	-16.915	-15.974	1.00	0.21
ATOM	2258	O	PRO	152	2.378	-16.371	-16.038	1.00	0.20
ATOM	2259	N	ASP	153	3.582	-18.209	-16.090	1.00	0.23
ATOM	2260	HN	ASP	153	4.468	-18.622	-16.031	1.00	0.25
ATOM	2261	CA	ASP	153	2.380	-19.063	-16.304	1.00	0.23
ATOM	2262	HA	ASP	153	1.890	-18.772	-17.221	1.00	0.23
ATOM	2263	CB	ASP	153	2.813	-20.526	-16.401	1.00	0.25
ATOM	2264	HB1	ASP	153	1.943	-21.163	-16.363	1.00	0.26
ATOM	2265	HB2	ASP	153	3.470	-20.762	-15.576	1.00	0.26
ATOM	2266	CG	ASP	153	3.550	-20.752	-17.722	1.00	0.27
ATOM	2267	OD1	ASP	153	4.768	-20.687	-17.717	1.00	1.08
ATOM	2268	OD2	ASP	153	2.884	-20.994	-18.715	1.00	1.14
ATOM	2269	C	ASP	153	1.409	-18.899	-15.133	1.00	0.21
ATOM	2270	O	ASP	153	0.208	-18.858	-15.310	1.00	0.21
ATOM	2271	N	ASP	154	1.919	-18.820	-13.935	1.00	0.21
ATOM	2272	HN	ASP	154	2.891	-18.866	-13.813	1.00	0.22

ATOM	2273	CA	ASP	154	1.025	-18.678	-12.752	1.00	0.21
ATOM	2274	HA	ASP	154	0.431	-19.572	-12.641	1.00	0.22
ATOM	2275	CB	ASP	154	1.880	-18.474	-11.496	1.00	0.23
ATOM	2276	HB1	ASP	154	2.466	-17.572	-11.602	1.00	0.22
ATOM	2277	HB2	ASP	154	2.541	-19.319	-11.370	1.00	0.25
ATOM	2278	CG	ASP	154	0.975	-18.347	-10.267	1.00	0.25
ATOM	2279	OD1	ASP	154	1.276	-18.982	-9.269	1.00	1.13
ATOM	2280	OD2	ASP	154	0.004	-17.613	-10.340	1.00	1.07
ATOM	2281	C	ASP	154	0.102	-17.473	-12.943	1.00	0.19
ATOM	2282	O	ASP	154	-1.095	-17.564	-12.759	1.00	0.19
ATOM	2283	N	ASP	155	0.645	-16.345	-13.303	1.00	0.19
ATOM	2284	HN	ASP	155	1.613	-16.288	-13.443	1.00	0.21
ATOM	2285	CA	ASP	155	-0.210	-15.140	-13.496	1.00	0.19
ATOM	2286	HA	ASP	155	-0.843	-15.011	-12.631	1.00	0.20
ATOM	2287	CB	ASP	155	0.683	-13.909	-13.653	1.00	0.21
ATOM	2288	HB1	ASP	155	0.087	-13.067	-13.969	1.00	0.22
ATOM	2289	HB2	ASP	155	1.443	-14.113	-14.393	1.00	0.22
ATOM	2290	CG	ASP	155	1.351	-13.588	-12.315	1.00	0.24
ATOM	2291	OD1	ASP	155	2.355	-12.896	-12.327	1.00	1.07
ATOM	2292	OD2	ASP	155	0.845	-14.038	-11.300	1.00	1.14
ATOM	2293	C	ASP	155	-1.087	-15.300	-14.744	1.00	0.19
ATOM	2294	O	ASP	155	-2.240	-14.918	-14.750	1.00	0.19
ATOM	2295	N	VAL	156	-0.555	-15.850	-15.802	1.00	0.19
ATOM	2296	HN	VAL	156	0.379	-16.147	-15.787	1.00	0.19
ATOM	2297	CA	VAL	156	-1.372	-16.013	-17.041	1.00	0.21
ATOM	2298	HA	VAL	156	-1.726	-15.044	-17.362	1.00	0.22
ATOM	2299	CB	VAL	156	-0.519	-16.630	-18.148	1.00	0.23
ATOM	2300	HB	VAL	156	-0.034	-17.521	-17.776	1.00	0.23
ATOM	2301	CG1	VAL	156	-1.416	-16.995	-19.333	1.00	0.27
ATOM	2302	HG11	VAL	156	-2.273	-16.338	-19.348	1.00	1.00
ATOM	2303	HG12	VAL	156	-1.747	-18.018	-19.235	1.00	1.05
ATOM	2304	HG13	VAL	156	-0.861	-16.882	-20.253	1.00	1.05
ATOM	2305	CG2	VAL	156	0.535	-15.618	-18.600	1.00	0.26
ATOM	2306	HG21	VAL	156	0.990	-15.162	-17.733	1.00	1.07
ATOM	2307	HG22	VAL	156	0.067	-14.856	-19.204	1.00	1.05
ATOM	2308	HG23	VAL	156	1.293	-16.123	-19.180	1.00	1.00
ATOM	2309	C	VAL	156	-2.574	-16.919	-16.754	1.00	0.20
ATOM	2310	O	VAL	156	-3.694	-16.615	-17.107	1.00	0.21
ATOM	2311	N	GLN	157	-2.356	-18.035	-16.124	1.00	0.20
ATOM	2312	HN	GLN	157	-1.447	-18.277	-15.847	1.00	0.20
ATOM	2313	CA	GLN	157	-3.498	-18.941	-15.824	1.00	0.22
ATOM	2314	HA	GLN	157	-3.987	-19.214	-16.747	1.00	0.24
ATOM	2315	CB	GLN	157	-2.995	-20.204	-15.117	1.00	0.24
ATOM	2316	HB1	GLN	157	-3.838	-20.774	-14.756	1.00	0.26
ATOM	2317	HB2	GLN	157	-2.368	-19.922	-14.282	1.00	0.23
ATOM	2318	CG	GLN	157	-2.184	-21.064	-16.095	1.00	0.25
ATOM	2319	HG1	GLN	157	-1.174	-20.686	-16.152	1.00	0.94
ATOM	2320	HG2	GLN	157	-2.636	-21.032	-17.074	1.00	0.87
ATOM	2321	CD	GLN	157	-2.152	-22.510	-15.598	1.00	1.19
ATOM	2322	OE1	GLN	157	-2.594	-22.799	-14.504	1.00	1.89
ATOM	2323	NE2	GLN	157	-1.646	-23.437	-16.364	1.00	1.96
ATOM	2324	HE21	GLN	157	-1.291	-23.203	-17.247	1.00	2.18
ATOM	2325	HE22	GLN	157	-1.624	-24.368	-16.058	1.00	2.65
ATOM	2326	C	GLN	157	-4.505	-18.214	-14.925	1.00	0.22
ATOM	2327	O	GLN	157	-5.702	-18.356	-15.077	1.00	0.24
ATOM	2328	N	GLY	158	-4.027	-17.456	-13.974	1.00	0.21
ATOM	2329	HN	GLY	158	-3.057	-17.370	-13.859	1.00	0.20
ATOM	2330	CA	GLY	158	-4.952	-16.741	-13.045	1.00	0.22
ATOM	2331	HA1	GLY	158	-4.380	-16.319	-12.232	1.00	0.22
ATOM	2332	HA2	GLY	158	-5.667	-17.446	-12.646	1.00	0.25
ATOM	2333	C	GLY	158	-5.704	-15.615	-13.766	1.00	0.20
ATOM	2334	O	GLY	158	-6.918	-15.552	-13.730	1.00	0.21
ATOM	2335	N	ILE	159	-5.007	-14.713	-14.405	1.00	0.18
ATOM	2336	HN	ILE	159	-4.028	-14.763	-14.418	1.00	0.18
ATOM	2337	CA	ILE	159	-5.713	-13.593	-15.097	1.00	0.19
ATOM	2338	HA	ILE	159	-6.301	-13.054	-14.375	1.00	0.20
ATOM	2339	CB	ILE	159	-4.679	-12.648	-15.735	1.00	0.19
ATOM	2340	HB	ILE	159	-3.950	-12.367	-14.988	1.00	0.20
ATOM	2341	CG1	ILE	159	-5.355	-11.384	-16.284	1.00	0.24
ATOM	2342	HG11	ILE	159	-6.308	-11.645	-16.717	1.00	0.26
ATOM	2343	HG12	ILE	159	-4.725	-10.952	-17.045	1.00	0.28
ATOM	2344	CG2	ILE	159	-3.968	-13.361	-16.880	1.00	0.21
ATOM	2345	HG21	ILE	159	-2.998	-12.914	-17.036	1.00	1.01
ATOM	2346	HG22	ILE	159	-4.556	-13.274	-17.781	1.00	1.01
ATOM	2347	HG23	ILE	159	-3.848	-14.398	-16.628	1.00	1.04
ATOM	2348	CD1	ILE	159	-5.571	-10.356	-15.166	1.00	0.27
ATOM	2349	HD11	ILE	159	-6.322	-9.644	-15.476	1.00	1.05

ATOM	2350	HD12	ILE	159	-4.644	-9.838	-14.978	1.00	1.06
ATOM	2351	HD13	ILE	159	-5.893	-10.848	-14.265	1.00	1.02
ATOM	2352	C	ILE	159	-6.644	-14.162	-16.173	1.00	0.21
ATOM	2353	O	ILE	159	-7.754	-13.700	-16.347	1.00	0.23
ATOM	2354	N	GLN	160	-6.215	-15.168	-16.885	1.00	0.22
ATOM	2355	HN	GLN	160	-5.322	-15.538	-16.726	1.00	0.21
ATOM	2356	CA	GLN	160	-7.097	-15.763	-17.930	1.00	0.27
ATOM	2357	HA	GLN	160	-7.457	-14.979	-18.580	1.00	0.29
ATOM	2358	CB	GLN	160	-6.317	-16.786	-18.756	1.00	0.31
ATOM	2359	HB1	GLN	160	-6.999	-17.334	-19.389	1.00	0.35
ATOM	2360	HB2	GLN	160	-5.809	-17.472	-18.093	1.00	0.30
ATOM	2361	CG	GLN	160	-5.289	-16.062	-19.626	1.00	0.34
ATOM	2362	HG1	GLN	160	-4.606	-15.512	-18.997	1.00	0.92
ATOM	2363	HG2	GLN	160	-5.799	-15.378	-20.290	1.00	0.91
ATOM	2364	CD	GLN	160	-4.508	-17.087	-20.451	1.00	1.11
ATOM	2365	OE1	GLN	160	-4.451	-18.248	-20.100	1.00	1.88
ATOM	2366	NE2	GLN	160	-3.901	-16.704	-21.540	1.00	1.83
ATOM	2367	HE21	GLN	160	-3.947	-15.767	-21.824	1.00	2.13
ATOM	2368	HE22	GLN	160	-3.398	-17.353	-22.075	1.00	2.46
ATOM	2369	C	GLN	160	-8.290	-16.447	-17.261	1.00	0.28
ATOM	2370	O	GLN	160	-9.386	-16.449	-17.779	1.00	0.31
ATOM	2371	N	SER	161	-8.086	-17.035	-16.117	1.00	0.27
ATOM	2372	HN	SER	161	-7.193	-17.030	-15.714	1.00	0.25
ATOM	2373	CA	SER	161	-9.213	-17.718	-15.424	1.00	0.30
ATOM	2374	HA	SER	161	-9.658	-18.444	-16.089	1.00	0.34
ATOM	2375	CB	SER	161	-8.690	-18.427	-14.174	1.00	0.33
ATOM	2376	HB1	SER	161	-7.861	-19.067	-14.444	1.00	0.35
ATOM	2377	HB2	SER	161	-9.476	-19.024	-13.741	1.00	0.36
ATOM	2378	OG	SER	161	-8.267	-17.455	-13.227	1.00	0.33
ATOM	2379	HG	SER	161	-9.045	-16.986	-12.915	1.00	0.94
ATOM	2380	C	SER	161	-10.267	-16.684	-15.019	1.00	0.30
ATOM	2381	O	SER	161	-11.433	-16.997	-14.882	1.00	0.35
ATOM	2382	N	LEU	162	-9.867	-15.457	-14.815	1.00	0.27
ATOM	2383	HN	LEU	162	-8.920	-15.225	-14.921	1.00	0.26
ATOM	2384	CA	LEU	162	-10.852	-14.413	-14.405	1.00	0.29
ATOM	2385	HA	LEU	162	-11.637	-14.869	-13.821	1.00	0.33
ATOM	2386	CB	LEU	162	-10.141	-13.350	-13.563	1.00	0.28
ATOM	2387	HB1	LEU	162	-10.802	-12.509	-13.411	1.00	0.29
ATOM	2388	HB2	LEU	162	-9.256	-13.017	-14.086	1.00	0.27
ATOM	2389	CG	LEU	162	-9.736	-13.937	-12.206	1.00	0.30
ATOM	2390	HG	LEU	162	-9.157	-14.836	-12.367	1.00	0.30
ATOM	2391	CD1	LEU	162	-8.883	-12.918	-11.450	1.00	0.33
ATOM	2392	HD11	LEU	162	-8.496	-13.370	-10.549	1.00	1.03
ATOM	2393	HD12	LEU	162	-9.490	-12.063	-11.191	1.00	1.01
ATOM	2394	HD13	LEU	162	-8.062	-12.601	-12.075	1.00	1.12
ATOM	2395	CD2	LEU	162	-10.980	-14.272	-11.374	1.00	0.33
ATOM	2396	HD21	LEU	162	-11.227	-15.315	-11.502	1.00	1.05
ATOM	2397	HD22	LEU	162	-11.812	-13.664	-11.697	1.00	1.09
ATOM	2398	HD23	LEU	162	-10.776	-14.078	-10.332	1.00	1.01
ATOM	2399	C	LEU	162	-11.461	-13.742	-15.643	1.00	0.30
ATOM	2400	O	LEU	162	-12.664	-13.615	-15.757	1.00	0.36
ATOM	2401	N	TYR	163	-10.645	-13.300	-16.564	1.00	0.27
ATOM	2402	HN	TYR	163	-9.677	-13.404	-16.452	1.00	0.26
ATOM	2403	CA	TYR	163	-11.188	-12.626	-17.783	1.00	0.31
ATOM	2404	HA	TYR	163	-12.144	-12.182	-17.549	1.00	0.33
ATOM	2405	CB	TYR	163	-10.219	-11.531	-18.236	1.00	0.29
ATOM	2406	HB1	TYR	163	-10.562	-11.112	-19.170	1.00	0.32
ATOM	2407	HB2	TYR	163	-9.234	-11.952	-18.371	1.00	0.29
ATOM	2408	CG	TYR	163	-10.162	-10.444	-17.190	1.00	0.25
ATOM	2409	CD1	TYR	163	-9.223	-10.520	-16.155	1.00	0.23
ATOM	2410	HD1	TYR	163	-8.545	-11.359	-16.103	1.00	0.23
ATOM	2411	CD2	TYR	163	-11.042	-9.357	-17.258	1.00	0.27
ATOM	2412	HD2	TYR	163	-11.767	-9.298	-18.056	1.00	0.30
ATOM	2413	CE1	TYR	163	-9.164	-9.511	-15.187	1.00	0.24
ATOM	2414	HE1	TYR	163	-8.439	-9.571	-14.388	1.00	0.25
ATOM	2415	CE2	TYR	163	-10.984	-8.348	-16.289	1.00	0.27
ATOM	2416	HE2	TYR	163	-11.663	-7.510	-16.340	1.00	0.30
ATOM	2417	CZ	TYR	163	-10.044	-8.425	-15.253	1.00	0.27
ATOM	2418	OH	TYR	163	-9.985	-7.430	-14.299	1.00	0.31
ATOM	2419	HH	TYR	163	-10.344	-7.782	-13.481	1.00	0.99
ATOM	2420	C	TYR	163	-11.367	-13.647	-18.909	1.00	0.37
ATOM	2421	O	TYR	163	-11.953	-13.357	-19.933	1.00	0.43
ATOM	2422	N	GLY	164	-10.865	-14.836	-18.729	1.00	0.38
ATOM	2423	HN	GLY	164	-10.394	-15.046	-17.896	1.00	0.35
ATOM	2424	CA	GLY	164	-11.001	-15.877	-19.789	1.00	0.47
ATOM	2425	HA1	GLY	164	-11.851	-15.651	-20.413	1.00	0.53

ATOM	2427	C	GLY	164	-9.735	-15.902	-20.648	1.00	0.55
ATOM	2428	O	GLY	164	-9.761	-15.580	-21.819	1.00	1.01
TER	2429		GLY	164					
HETATM	2430	ZN	ZN	166	-0.218	-6.515	-2.613	1.00	0.24
HETATM	2431	ZN	ZN	167	-3.506	6.833	-0.714	1.00	0.97
HETATM	2432	CA	CA	168	6.060	3.350	3.030	1.00	0.23
HETATM	2433	C1	WAY	169	2.180	-4.315	1.627	0.00	0.30
HETATM	2434	C2	WAY	169	0.865	-4.629	1.215	0.00	0.33
HETATM	2435	1CE1	WAY	169	-0.170	-4.517	2.143	0.00	0.38
HETATM	2436	1CZ	WAY	169	0.074	-4.157	3.457	0.00	0.40
HETATM	2437	1CE2	WAY	169	1.355	-3.807	3.841	0.00	0.38
HETATM	2438	C6	WAY	169	2.395	-3.805	2.922	0.00	0.33
HETATM	2439	1HE1	WAY	169	-1.190	-4.713	1.839	0.00	0.42
HETATM	2440	1HZ	WAY	169	-0.734	-4.151	4.173	0.00	0.45
HETATM	2441	1HE2	WAY	169	1.535	-3.534	4.872	0.00	0.42
HETATM	2442	C10	WAY	169	0.444	-5.080	-0.136	0.00	0.36
HETATM	2443	O11	WAY	169	0.467	-6.264	-0.463	0.00	0.58
HETATM	2444	N12	WAY	169	-0.019	-4.195	-1.032	0.00	0.61
HETATM	2445	O13	WAY	169	-0.045	-4.608	-2.371	0.00	0.68
HETATM	2446	H14	WAY	169	-0.357	-3.297	-0.743	0.00	0.88
HETATM	2447	H15	WAY	169	-0.953	-4.727	-2.645	0.00	1.13
HETATM	2448	1CH1	WAY	169	3.728	-3.247	3.360	0.00	0.37
HETATM	2449	1HH1	WAY	169	3.702	-2.162	3.422	0.00	1.07
HETATM	2450	1HH2	WAY	169	4.519	-3.516	2.664	0.00	1.06
HETATM	2451	1HH3	WAY	169	4.013	-3.623	4.339	0.00	1.11
HETATM	2452	N20	WAY	169	3.274	-4.485	0.819	0.00	0.29
HETATM	2453	S21	WAY	169	3.865	-3.175	0.021	0.00	0.25
HETATM	2454	2CB	WAY	169	3.882	-5.812	0.684	0.00	0.32
HETATM	2455	2CE1	WAY	169	7.334	-6.241	2.178	0.00	1.09
HETATM	2456	2CZ	WAY	169	6.971	-6.520	3.488	0.00	0.53
HETATM	2457	N25	WAY	169	5.697	-6.659	3.876	0.00	1.47
HETATM	2458	2CD2	WAY	169	4.747	-6.451	2.954	0.00	1.37
HETATM	2459	C27	WAY	169	5.010	-6.084	1.640	0.00	0.36
HETATM	2460	2CD1	WAY	169	6.338	-5.982	1.250	0.00	1.14
HETATM	2461	2HE1	WAY	169	8.374	-6.224	1.881	0.00	1.94
HETATM	2462	2HZ	WAY	169	7.752	-6.630	4.227	0.00	0.61
HETATM	2463	2HD2	WAY	169	3.708	-6.570	3.227	0.00	2.23
HETATM	2464	2HD1	WAY	169	6.599	-5.706	0.239	0.00	2.05
HETATM	2465	2HB1	WAY	169	4.245	-5.905	-0.339	0.00	0.31
HETATM	2466	2HB2	WAY	169	3.095	-6.552	0.832	0.00	0.34
HETATM	2467	C35	WAY	169	4.187	-3.617	-1.665	0.00	0.23
HETATM	2468	3CD1	WAY	169	3.310	-3.216	-2.661	0.00	0.25
HETATM	2469	3CE1	WAY	169	3.622	-3.465	-3.992	0.00	0.27
HETATM	2470	C38	WAY	169	4.769	-4.183	-4.326	0.00	0.24
HETATM	2471	3CE2	WAY	169	5.602	-4.644	-3.308	0.00	0.23
HETATM	2472	3CD2	WAY	169	5.315	-4.359	-1.979	0.00	0.23
HETATM	2473	3HD1	WAY	169	2.392	-2.714	-2.389	0.00	0.29
HETATM	2474	3HE1	WAY	169	2.961	-3.091	-4.758	0.00	0.31
HETATM	2475	3HE2	WAY	169	6.481	-5.228	-3.535	0.00	0.26
HETATM	2476	3HD2	WAY	169	5.959	-4.707	-1.184	0.00	0.27
HETATM	2477	O45	WAY	169	5.078	-4.439	-5.664	0.00	0.27
HETATM	2478	3CH	WAY	169	6.245	-5.202	-5.904	0.00	0.28
HETATM	2479	3HH1	WAY	169	6.379	-5.372	-6.973	0.00	0.31
HETATM	2480	3HH2	WAY	169	6.178	-6.172	-5.407	0.00	0.28
HETATM	2481	3HH3	WAY	169	7.127	-4.683	-5.526	0.00	0.29
HETATM	2482	O50	WAY	169	5.123	-2.847	0.614	0.00	0.27
HETATM	2483	O51	WAY	169	2.834	-2.186	0.004	0.00	0.25

END

		Atom Type	Res.		X	Y	Z	Occ.	B	MOL.
ATOM	1	CB	THR	7	73.468	27.410	6.079	1.00	42.70	A_13
ATOM	2	OG1	THR	7	72.149	27.911	6.358	1.00	37.82	A_13
ATOM	4	CG2	THR	7	73.843	26.297	7.068	1.00	25.79	A_13
ATOM	5	C	THR	7	75.936	28.076	6.227	1.00	28.29	A_13
ATOM	6	O	THR	7	76.497	28.090	7.332	1.00	22.94	A_13
ATOM	9	N	THR	7	74.360	29.396	4.862	1.00	20.25	A_13
ATOM	11	CA	THR	7	74.501	28.593	6.099	1.00	21.49	A_13
ATOM	12	N	LEU	8	76.547	27.691	5.099	1.00	32.90	A_13
ATOM	14	CA	LEU	8	77.915	27.150	5.105	1.00	31.85	A_13
ATOM	15	CB	LEU	8	77.952	25.759	4.438	1.00	21.38	A_13
ATOM	16	CG	LEU	8	78.016	25.576	2.910	1.00	29.31	A_13
ATOM	17	CD1	LEU	8	79.463	25.509	2.425	1.00	16.78	A_13
ATOM	18	CD2	LEU	8	77.334	24.292	2.527	1.00	23.37	A_13
ATOM	19	C	LEU	8	78.956	28.070	4.465	1.00	24.01	A_13
ATOM	20	O	LEU	8	78.835	28.415	3.293	1.00	26.18	A_13
ATOM	21	N	LYS	9	79.980	28.424	5.251	1.00	36.26	A_13
ATOM	23	CA	LYS	9	81.106	29.298	4.867	1.00	23.24	A_13
ATOM	24	CB	LYS	9	82.438	28.521	4.977	1.00	25.52	A_13
ATOM	25	CG	LYS	9	82.767	27.570	3.815	1.00	19.05	A_13
ATOM	26	CD	LYS	9	83.661	28.243	2.753	1.00	31.69	A_13
ATOM	27	CE	LYS	9	83.451	27.688	1.323	1.00	25.30	A_13
ATOM	28	NZ	LYS	9	82.056	27.938	0.797	1.00	20.65	A_13
ATOM	32	C	LYS	9	81.042	30.073	3.526	1.00	31.41	A_13
ATOM	33	O	LYS	9	80.764	29.505	2.466	1.00	22.31	A_13
ATOM	34	N	TRP	10	81.327	31.372	3.573	1.00	15.84	A_13
ATOM	36	CA	TRP	10	81.312	32.172	2.361	1.00	10.58	A_13
ATOM	37	CB	TRP	10	81.636	33.620	2.680	1.00	21.39	A_13
ATOM	38	CG	TRP	10	80.529	34.337	3.343	1.00	22.84	A_13
ATOM	39	CD2	TRP	10	79.479	35.074	2.697	1.00	20.41	A_13
ATOM	40	CE2	TRP	10	78.676	35.631	3.718	1.00	24.50	A_13
ATOM	41	CE3	TRP	10	79.142	35.320	1.357	1.00	13.29	A_13
ATOM	42	CD1	TRP	10	80.327	34.469	4.682	1.00	13.40	A_13
ATOM	43	NE1	TRP	10	79.220	35.253	4.919	1.00	18.40	A_13
ATOM	45	CZ2	TRP	10	77.550	36.418	3.442	1.00	12.63	A_13
ATOM	46	CZ3	TRP	10	78.021	36.105	1.083	1.00	19.89	A_13
ATOM	47	CH2	TRP	10	77.242	36.641	2.120	1.00	13.62	A_13
ATOM	48	C	TRP	10	82.377	31.594	1.455	1.00	22.95	A_13
ATOM	49	O	TRP	10	83.450	31.221	1.920	1.00	16.28	A_13
ATOM	50	N	SER	11	82.087	31.533	0.167	1.00	14.81	A_13
ATOM	52	CA	SER	11	83.017	30.975	-0.801	1.00	19.50	A_13
ATOM	53	CB	SER	11	82.282	30.596	-2.086	1.00	24.36	A_13
ATOM	54	OG	SER	11	81.605	29.353	-1.958	1.00	40.49	A_13
ATOM	56	C	SER	11	84.190	31.867	-1.134	1.00	16.53	A_13
ATOM	57	O	SER	11	85.132	31.423	-1.779	1.00	23.48	A_13
ATOM	58	N	LYS	12	84.153	33.113	-0.686	1.00	12.50	A_13
ATOM	60	CA	LYS	12	85.232	34.057	-0.961	1.00	17.05	A_13
ATOM	61	CB	LYS	12	84.741	35.168	-1.891	1.00	17.32	A_13
ATOM	62	CG	LYS	12	83.526	35.898	-1.350	1.00	18.49	A_13
ATOM	63	CD	LYS	12	82.788	36.644	-2.446	1.00	18.29	A_13
ATOM	64	CE	LYS	12	81.534	37.282	-1.888	1.00	18.44	A_13
ATOM	65	NZ	LYS	12	80.805	38.094	-2.895	1.00	16.65	A_13
ATOM	69	C	LYS	12	85.687	34.662	0.344	1.00	11.16	A_13
ATOM	70	O	LYS	12	84.946	34.637	1.319	1.00	12.63	A_13
ATOM	71	N	MET	13	86.915	35.185	0.355	1.00	15.52	A_13
ATOM	73	CA	MET	13	87.516	35.801	1.537	1.00	11.04	A_13
ATOM	74	CB	MET	13	89.028	35.547	1.565	1.00	16.57	A_13
ATOM	75	CG	MET	13	89.431	34.082	1.707	1.00	20.92	A_13
ATOM	76	SD	MET	13	88.905	33.235	3.227	1.00	20.10	A_13
ATOM	77	CE	MET	13	87.486	32.313	2.604	1.00	16.29	A_13
ATOM	78	C	MET	13	87.258	37.296	1.572	1.00	13.23	A_13
ATOM	79	O	MET	13	87.247	37.916	2.634	1.00	22.80	A_13
ATOM	80	N	ASN	14	87.111	37.875	0.389	1.00	15.02	A_13
ATOM	82	CA	ASN	14	86.853	39.294	0.241	1.00	33.02	A_13
ATOM	83	CB	ASN	14	87.445	39.801	-1.082	1.00	19.42	A_13
ATOM	84	CG	ASN	14	88.925	39.482	-1.217	1.00	30.32	A_13
ATOM	85	OD1	ASN	14	89.343	38.341	-1.031	1.00	30.12	A_13
ATOM	86	ND2	ASN	14	89.723	40.489	-1.549	1.00	28.22	A_13
ATOM	89	C	ASN	14	85.337	39.482	0.277	1.00	27.58	A_13
ATOM	90	O	ASN	14	84.606	38.935	-0.568	1.00	28.01	A_13
ATOM	91	N	LEU	15	84.868	40.212	1.287	1.00	19.06	A_13
ATOM	93	CA	LEU	15	83.444	40.450	1.459	1.00	20.03	A_13
ATOM	94	CB	LEU	15	82.930	39.690	2.691	1.00	19.55	A_13
ATOM	95	CG	LEU	15	83.027	38.166	2.593	1.00	19.02	A_13
ATOM	96	CD1	LEU	15	83.216	37.555	3.962	1.00	17.48	A_13
ATOM	97	CD2	LEU	15	81.799	37.604	1.903	1.00	23.43	A_13
ATOM	98	C	LEU	15	83.161	41.928	1.609	1.00	19.52	A_13
ATOM	99	O	LEU	15	83.980	42.676	2.130	1.00	15.98	A_13

FIG. 5

ATOM	100	N	THR	16	81.983	42.343	1.162	1.00	21.22	A_13
ATOM	102	CA	THR	16	81.578	43.736	1.252	1.00	10.00	A_13
ATOM	103	CB	THR	16	81.194	44.257	-0.109	1.00	10.00	A_13
ATOM	104	OG1	THR	16	80.225	43.370	-0.681	1.00	22.43	A_13
ATOM	106	CG2	THR	16	82.427	44.383	-1.009	1.00	15.42	A_13
ATOM	107	C	THR	16	80.368	43.869	2.184	1.00	14.48	A_13
ATOM	108	O	THR	16	79.647	42.897	2.445	1.00	15.74	A_13
ATOM	109	N	TYR	17	80.176	45.065	2.716	1.00	15.89	A_13
ATOM	111	CA	TYR	17	79.064	45.340	3.604	1.00	13.19	A_13
ATOM	112	CB	TYR	17	79.480	45.195	5.067	1.00	21.42	A_13
ATOM	113	CG	TYR	17	80.448	46.236	5.580	1.00	26.23	A_13
ATOM	114	CD1	TYR	17	81.824	46.081	5.412	1.00	16.37	A_13
ATOM	115	CE1	TYR	17	82.724	46.981	5.988	1.00	12.90	A_13
ATOM	116	CD2	TYR	17	79.990	47.329	6.331	1.00	17.15	A_13
ATOM	117	CE2	TYR	17	80.880	48.235	6.912	1.00	24.15	A_13
ATOM	118	CZ	TYR	17	82.244	48.057	6.743	1.00	23.38	A_13
ATOM	119	OH	TYR	17	83.121	48.942	7.343	1.00	19.47	A_13
ATOM	121	C	TYR	17	78.573	46.740	3.343	1.00	10.00	A_13
ATOM	122	O	TYR	17	79.298	47.559	2.782	1.00	19.27	A_13
ATOM	123	N	ARG	18	77.349	47.019	3.762	1.00	18.52	A_13
ATOM	125	CA	ARG	18	76.762	48.332	3.577	1.00	10.00	A_13
ATOM	126	CB	ARG	18	75.970	48.363	2.274	1.00	10.00	A_13
ATOM	127	CG	ARG	18	75.134	49.619	2.094	1.00	14.01	A_13
ATOM	128	CD	ARG	18	74.266	49.524	0.846	1.00	13.91	A_13
ATOM	129	NE	ARG	18	73.298	50.615	0.782	1.00	13.55	A_13
ATOM	131	CZ	ARG	18	72.165	50.571	0.092	1.00	10.00	A_13
ATOM	132	NH1	ARG	18	71.855	49.488	-0.602	1.00	14.30	A_13
ATOM	135	NH2	ARG	18	71.331	51.604	0.125	1.00	28.79	A_13
ATOM	138	C	ARG	18	75.842	48.640	4.741	1.00	10.65	A_13
ATOM	139	O	ARG	18	75.037	47.796	5.141	1.00	12.86	A_13
ATOM	140	N	ILE	19	76.014	49.814	5.332	1.00	25.54	A_13
ATOM	142	CA	ILE	19	75.169	50.265	6.436	1.00	24.52	A_13
ATOM	143	CB	ILE	19	75.944	51.236	7.350	1.00	18.37	A_13
ATOM	144	CG2	ILE	19	75.034	51.765	8.485	1.00	13.87	A_13
ATOM	145	CG1	ILE	19	77.204	50.545	7.888	1.00	27.67	A_13
ATOM	146	CD1	ILE	19	78.203	51.501	8.557	1.00	22.81	A_13
ATOM	147	C	ILE	19	74.062	51.027	5.698	1.00	21.11	A_13
ATOM	148	O	ILE	19	74.261	52.179	5.300	1.00	10.00	A_13
ATOM	149	N	VAL	20	72.916	50.378	5.487	1.00	19.76	A_13
ATOM	151	CA	VAL	20	71.829	51.014	4.735	1.00	18.20	A_13
ATOM	152	CB	VAL	20	70.774	49.983	4.193	1.00	15.42	A_13
ATOM	153	CG1	VAL	20	71.384	48.570	4.088	1.00	10.00	A_13
ATOM	154	CG2	VAL	20	69.496	50.030	4.992	1.00	18.62	A_13
ATOM	155	C	VAL	20	71.175	52.206	5.443	1.00	11.67	A_13
ATOM	156	O	VAL	20	70.652	53.110	4.798	1.00	18.36	A_13
ATOM	157	N	ASN	21	71.153	52.187	6.773	1.00	10.94	A_13
ATOM	159	CA	ASN	21	70.609	53.316	7.544	1.00	11.99	A_13
ATOM	160	CB	ASN	21	69.078	53.307	7.675	1.00	10.00	A_13
ATOM	161	CG	ASN	21	68.533	51.978	8.107	1.00	14.93	A_13
ATOM	162	OD1	ASN	21	67.627	51.449	7.486	1.00	21.54	A_13
ATOM	163	ND2	ASN	21	69.105	51.408	9.148	1.00	10.00	A_13
ATOM	166	C	ASN	21	71.291	53.382	8.897	1.00	18.90	A_13
ATOM	167	O	ASN	21	72.006	52.447	9.283	1.00	12.49	A_13
ATOM	168	N	TYR	22	71.053	54.471	9.618	1.00	17.47	A_13
ATOM	170	CA	TYR	22	71.681	54.708	10.910	1.00	24.85	A_13
ATOM	171	CB	TYR	22	72.556	55.954	10.818	1.00	13.52	A_13
ATOM	172	CG	TYR	22	73.791	55.748	9.991	1.00	10.00	A_13
ATOM	173	CD1	TYR	22	75.033	55.600	10.598	1.00	14.05	A_13
ATOM	174	CE1	TYR	22	76.180	55.370	9.841	1.00	13.69	A_13
ATOM	175	CD2	TYR	22	73.717	55.663	8.608	1.00	10.00	A_13
ATOM	176	CE2	TYR	22	74.848	55.432	7.847	1.00	17.10	A_13
ATOM	177	CZ	TYR	22	76.077	55.288	8.476	1.00	14.43	A_13
ATOM	178	OH	TYR	22	77.204	55.072	7.737	1.00	10.00	A_13
ATOM	180	C	TYR	22	70.726	54.862	12.076	1.00	25.95	A_13
ATOM	181	O	TYR	22	69.593	55.311	11.916	1.00	10.00	A_13
ATOM	182	N	THR	23	71.187	54.483	13.259	1.00	20.30	A_13
ATOM	184	CA	THR	23	70.367	54.606	14.450	1.00	29.11	A_13
ATOM	185	CB	THR	23	70.821	53.635	15.584	1.00	10.90	A_13
ATOM	186	OG1	THR	23	70.136	53.968	16.792	1.00	10.00	A_13
ATOM	188	CG2	THR	23	72.328	53.752	15.852	1.00	16.51	A_13
ATOM	189	C	THR	23	70.459	56.038	14.959	1.00	18.14	A_13
ATOM	190	O	THR	23	71.360	56.785	14.575	1.00	10.00	A_13
ATOM	191	N	PRO	24	69.433	56.487	15.691	1.00	12.76	A_13
ATOM	192	CD	PRO	24	68.061	55.950	15.716	1.00	15.26	A_13
ATOM	193	CA	PRO	24	69.453	57.844	16.232	1.00	22.70	A_13
ATOM	194	CB	PRO	24	67.985	58.086	16.585	1.00	28.52	A_13
ATOM	195	CG	PRO	24	67.448	56.706	16.841	1.00	15.78	A_13

```
ATOM    196  C   PRO   24      70.346  57.945  17.475  1.00 24.52      A_13
ATOM    197  O   PRO   24      70.790  59.040  17.831  1.00 10.00      A_13
ATOM    198  N   ASP   25      70.614  56.797  18.105  1.00 11.82      A_13
ATOM    200  CA  ASP   25      71.416  56.721  19.336  1.00 12.31      A_13
ATOM    201  CB  ASP   25      71.339  55.317  19.917  1.00 25.26      A_13
ATOM    202  CG  ASP   25      69.927  54.782  19.977  1.00 10.00      A_13
ATOM    203  OD1 ASP   25      69.783  53.567  20.159  1.00 20.90      A_13
ATOM    204  OD2 ASP   25      68.960  55.558  19.841  1.00 18.45      A_13
ATOM    205  C   ASP   25      72.891  57.113  19.286  1.00 14.34      A_13
ATOM    206  O   ASP   25      73.449  57.511  20.301  1.00 11.77      A_13
ATOM    207  N   MET   26      73.546  56.873  18.157  1.00 20.78      A_13
ATOM    209  CA  MET   26      74.960  57.208  18.010  1.00 20.03      A_13
ATOM    210  CB  MET   26      75.791  55.928  17.916  1.00 13.86      A_13
ATOM    211  CG  MET   26      75.966  55.181  19.231  1.00 19.00      A_13
ATOM    212  SD  MET   26      76.043  53.404  18.941  1.00 14.67      A_13
ATOM    213  CE  MET   26      77.737  53.223  18.385  1.00 19.74      A_13
ATOM    214  C   MET   26      75.157  58.047  16.754  1.00 13.32      A_13
ATOM    215  O   MET   26      74.274  58.086  15.900  1.00 16.81      A_13
ATOM    216  N   THR   27      76.285  58.749  16.656  1.00 10.29      A_13
ATOM    218  CA  THR   27      76.568  59.564  15.470  1.00 17.00      A_13
ATOM    219  CB  THR   27      77.710  60.596  15.700  1.00 11.79      A_13
ATOM    220  OG1 THR   27      78.969  59.921  15.729  1.00 23.77      A_13
ATOM    222  CG2 THR   27      77.519  61.342  17.020  1.00 21.98      A_13
ATOM    223  C   THR   27      76.996  58.634  14.347  1.00 13.37      A_13
ATOM    224  O   THR   27      77.411  57.500  14.608  1.00 11.05      A_13
ATOM    225  N   HIS   28      76.972  59.124  13.113  1.00 10.00      A_13
ATOM    227  CA  HIS   28      77.362  58.300  11.980  1.00 10.96      A_13
ATOM    228  CB  HIS   28      77.240  59.071  10.657  1.00 16.07      A_13
ATOM    229  CG  HIS   28      75.829  59.382  10.264  1.00 15.53      A_13
ATOM    230  CD2 HIS   28      74.707  59.531  11.016  1.00 21.47      A_13
ATOM    231  ND1 HIS   28      75.440  59.597   8.959  1.00 30.32      A_13
ATOM    233  CE1 HIS   28      74.149  59.868   8.920  1.00 19.38      A_13
ATOM    234  NE2 HIS   28      73.680  59.833  10.160  1.00 29.43      A_13
ATOM    236  C   HIS   28      78.769  57.735  12.151  1.00 14.80      A_13
ATOM    237  O   HIS   28      79.005  56.568  11.851  1.00 28.24      A_13
ATOM    238  N   SER   29      79.703  58.548  12.634  1.00 14.00      A_13
ATOM    240  CA  SER   29      81.068  58.070  12.854  1.00 19.57      A_13
ATOM    241  CB  SER   29      82.001  59.219  13.242  1.00 17.84      A_13
ATOM    242  OG  SER   29      82.383  59.936  12.084  1.00 28.25      A_13
ATOM    244  C   SER   29      81.134  56.983  13.917  1.00 15.23      A_13
ATOM    245  O   SER   29      81.818  55.973  13.733  1.00 13.73      A_13
ATOM    246  N   GLU   30      80.428  57.182  15.027  1.00 27.71      A_13
ATOM    248  CA  GLU   30      80.430  56.186  16.100  1.00 23.60      A_13
ATOM    249  CB  GLU   30      79.571  56.635  17.289  1.00 21.72      A_13
ATOM    250  CG  GLU   30      80.048  57.913  17.973  1.00 24.07      A_13
ATOM    251  CD  GLU   30      79.205  58.279  19.185  1.00 21.06      A_13
ATOM    252  OE1 GLU   30      79.784  58.660  20.218  1.00 46.95      A_13
ATOM    253  OE2 GLU   30      77.963  58.185  19.119  1.00 18.27      A_13
ATOM    254  C   GLU   30      79.895  54.877  15.553  1.00 18.75      A_13
ATOM    255  O   GLU   30      80.456  53.809  15.815  1.00 13.06      A_13
ATOM    256  N   VAL   31      78.839  54.970  14.746  1.00 16.23      A_13
ATOM    258  CA  VAL   31      78.225  53.781  14.146  1.00 22.33      A_13
ATOM    259  CB  VAL   31      76.899  54.135  13.390  1.00 23.53      A_13
ATOM    260  CG1 VAL   31      76.384  52.920  12.628  1.00 14.39      A_13
ATOM    261  CG2 VAL   31      75.829  54.587  14.377  1.00 10.00      A_13
ATOM    262  C   VAL   31      79.208  53.040  13.216  1.00 20.29      A_13
ATOM    263  O   VAL   31      79.330  51.814  13.282  1.00 14.02      A_13
ATOM    264  N   GLU   32      79.913  53.790  12.370  1.00 23.94      A_13
ATOM    266  CA  GLU   32      80.887  53.219  11.446  1.00 10.18      A_13
ATOM    267  CB  GLU   32      81.406  54.285  10.502  1.00 16.50      A_13
ATOM    268  CG  GLU   32      80.424  54.605   9.427  1.00 20.84      A_13
ATOM    269  CD  GLU   32      80.330  56.080   9.155  1.00 22.31      A_13
ATOM    270  OE1 GLU   32      79.285  56.509   8.639  1.00 29.39      A_13
ATOM    271  OE2 GLU   32      81.294  56.812   9.458  1.00 22.01      A_13
ATOM    272  C   GLU   32      82.056  52.565  12.137  1.00 18.93      A_13
ATOM    273  O   GLU   32      82.474  51.470  11.753  1.00 24.42      A_13
ATOM    274  N   LYS   33      82.610  53.241  13.139  1.00 19.78      A_13
ATOM    276  CA  LYS   33      83.726  52.661  13.873  1.00 28.68      A_13
ATOM    277  CB  LYS   33      84.340  53.681  14.837  1.00 18.54      A_13
ATOM    278  CG  LYS   33      85.016  54.855  14.135  1.00 31.19      A_13
ATOM    279  CD  LYS   33      86.135  54.425  13.148  1.00 40.31      A_13
ATOM    280  CE  LYS   33      85.600  53.972  11.785  1.00 21.99      A_13
ATOM    281  NZ  LYS   33      86.646  53.779  10.773  1.00 33.20      A_13
ATOM    285  C   LYS   33      83.242  51.407  14.594  1.00 12.66      A_13
ATOM    286  O   LYS   33      83.892  50.361  14.552  1.00 15.54      A_13
ATOM    287  N   ALA   34      82.036  51.481  15.148  1.00 20.70      A_13
ATOM    289  CA  ALA   34      81.453  50.344  15.843  1.00 10.00      A_13
```

ATOM	290	CB	ALA	34	80.040	50.651	16.279	1.00	18.59	A_13
ATOM	291	C	ALA	34	81.468	49.119	14.940	1.00	13.45	A_13
ATOM	292	O	ALA	34	82.067	48.095	15.284	1.00	15.90	A_13
ATOM	293	N	PHE	35	80.857	49.234	13.766	1.00	19.57	A_13
ATOM	295	CA	PHE	35	80.802	48.112	12.812	1.00	26.77	A_13
ATOM	296	CB	PHE	35	79.837	48.423	11.660	1.00	17.34	A_13
ATOM	297	CG	PHE	35	78.390	48.477	12.077	1.00	30.55	A_13
ATOM	298	CD1	PHE	35	77.838	47.464	12.863	1.00	26.58	A_13
ATOM	299	CD2	PHE	35	77.570	49.512	11.653	1.00	10.00	A_13
ATOM	300	CE1	PHE	35	76.494	47.485	13.212	1.00	12.45	A_13
ATOM	301	CE2	PHE	35	76.224	49.538	12.002	1.00	17.92	A_13
ATOM	302	CZ	PHE	35	75.684	48.525	12.777	1.00	13.29	A_13
ATOM	303	C	PHE	35	82.170	47.754	12.236	1.00	11.31	A_13
ATOM	304	O	PHE	35	82.493	46.573	12.034	1.00	11.37	A_13
ATOM	305	N	LYS	36	82.962	48.778	11.945	1.00	17.06	A_13
ATOM	307	CA	LYS	36	84.293	48.573	11.400	1.00	17.41	A_13
ATOM	308	CB	LYS	36	84.991	49.922	11.208	1.00	11.20	A_13
ATOM	309	CG	LYS	36	86.282	49.792	10.439	1.00	28.84	A_13
ATOM	310	CD	LYS	36	87.246	50.917	10.738	1.00	24.52	A_13
ATOM	311	CE	LYS	36	88.542	50.703	9.978	1.00	12.87	A_13
ATOM	312	NZ	LYS	36	88.264	50.536	8.514	1.00	23.69	A_13
ATOM	316	C	LYS	36	85.122	47.685	12.345	1.00	16.09	A_13
ATOM	317	O	LYS	36	85.701	46.686	11.938	1.00	21.50	A_13
ATOM	318	N	LYS	37	85.173	48.057	13.613	1.00	12.42	A_13
ATOM	320	CA	LYS	37	85.926	47.303	14.591	1.00	12.36	A_13
ATOM	321	CB	LYS	37	85.953	48.066	15.917	1.00	13.65	A_13
ATOM	322	CG	LYS	37	86.744	47.374	17.028	1.00	13.38	A_13
ATOM	323	CD	LYS	37	88.192	47.125	16.616	1.00	38.32	A_13
ATOM	324	CE	LYS	37	88.750	45.825	17.205	1.00	34.46	A_13
ATOM	325	NZ	LYS	37	88.234	44.576	16.557	1.00	12.49	A_13
ATOM	329	C	LYS	37	85.372	45.887	14.786	1.00	17.04	A_13
ATOM	330	O	LYS	37	86.131	44.958	15.053	1.00	18.14	A_13
ATOM	331	N	ALA	38	84.061	45.711	14.649	1.00	24.47	A_13
ATOM	333	CA	ALA	38	83.452	44.392	14.822	1.00	11.03	A_13
ATOM	334	CB	ALA	38	81.941	44.504	14.890	1.00	14.71	A_13
ATOM	335	C	ALA	38	83.900	43.451	13.697	1.00	20.27	A_13
ATOM	336	O	ALA	38	84.143	42.266	13.936	1.00	18.80	A_13
ATOM	337	N	PHE	39	84.021	43.971	12.477	1.00	22.58	A_13
ATOM	339	CA	PHE	39	84.492	43.158	11.355	1.00	18.87	A_13
ATOM	340	CB	PHE	39	84.350	43.899	10.027	1.00	19.91	A_13
ATOM	341	CG	PHE	39	82.993	43.783	9.414	1.00	10.00	A_13
ATOM	342	CD1	PHE	39	82.266	44.915	9.097	1.00	17.54	A_13
ATOM	343	CD2	PHE	39	82.438	42.533	9.143	1.00	15.92	A_13
ATOM	344	CE1	PHE	39	81.008	44.808	8.520	1.00	20.75	A_13
ATOM	345	CE2	PHE	39	81.186	42.418	8.569	1.00	10.00	A_13
ATOM	346	CZ	PHE	39	80.467	43.555	8.252	1.00	10.00	A_13
ATOM	347	C	PHE	39	85.955	42.827	11.589	1.00	16.52	A_13
ATOM	348	O	PHE	39	86.382	41.689	11.387	1.00	19.70	A_13
ATOM	349	N	LYS	40	86.699	43.822	12.072	1.00	21.31	A_13
ATOM	351	CA	LYS	40	88.117	43.673	12.369	1.00	20.07	A_13
ATOM	352	CB	LYS	40	88.703	44.967	12.927	1.00	13.77	A_13
ATOM	353	CG	LYS	40	90.192	44.885	13.171	1.00	11.54	A_13
ATOM	354	CD	LYS	40	90.757	46.242	13.507	1.00	10.34	A_13
ATOM	355	CE	LYS	40	92.236	46.142	13.838	1.00	11.24	A_13
ATOM	356	NZ	LYS	40	92.468	45.518	15.179	1.00	27.33	A_13
ATOM	360	C	LYS	40	88.352	42.534	13.337	1.00	12.06	A_13
ATOM	361	O	LYS	40	89.252	41.719	13.124	1.00	25.09	A_13
ATOM	362	N	VAL	41	87.495	42.418	14.349	1.00	12.26	A_13
ATOM	364	CA	VAL	41	87.630	41.331	15.325	1.00	17.89	A_13
ATOM	365	CB	VAL	41	86.351	41.205	16.216	1.00	10.00	A_13
ATOM	366	CG1	VAL	41	86.298	39.865	16.894	1.00	23.82	A_13
ATOM	367	CG2	VAL	41	86.329	42.274	17.259	1.00	17.65	A_13
ATOM	368	C	VAL	41	87.822	40.009	14.560	1.00	23.06	A_13
ATOM	369	O	VAL	41	88.664	39.168	14.912	1.00	11.82	A_13
ATOM	370	N	TRP	42	87.069	39.871	13.471	1.00	21.42	A_13
ATOM	372	CA	TRP	42	87.085	38.666	12.661	1.00	21.32	A_13
ATOM	373	CB	TRP	42	85.713	38.476	12.009	1.00	18.84	A_13
ATOM	374	CG	TRP	42	84.605	38.397	13.025	1.00	25.92	A_13
ATOM	375	CD2	TRP	42	84.437	37.369	14.024	1.00	16.65	A_13
ATOM	376	CE2	TRP	42	83.260	37.680	14.737	1.00	17.58	A_13
ATOM	377	CE3	TRP	42	85.165	36.223	14.380	1.00	11.14	A_13
ATOM	378	CD1	TRP	42	83.563	39.249	13.179	1.00	10.00	A_13
ATOM	379	NE1	TRP	42	82.755	38.832	14.200	1.00	10.91	A_13
ATOM	381	CZ2	TRP	42	82.785	36.879	15.793	1.00	14.81	A_13
ATOM	382	CZ3	TRP	42	84.691	35.425	15.436	1.00	23.68	A_13
ATOM	383	CH2	TRP	42	83.513	35.759	16.125	1.00	12.75	A_13
ATOM	384	C	TRP	42	88.190	38.600	11.623	1.00	27.45	A_13

ATOM	385	O	TRP	42	88.834	37.556	11.472	1.00	11.84	A_13
ATOM	386	N	SER	43	88.413	39.702	10.909	1.00	25.46	A_13
ATOM	388	CA	SER	43	89.449	39.740	9.881	1.00	19.61	A_13
ATOM	389	CB	SER	43	89.342	40.993	8.991	1.00	16.16	A_13
ATOM	390	OG	SER	43	89.495	42.199	9.709	1.00	26.34	A_13
ATOM	392	C	SER	43	90.837	39.615	10.491	1.00	11.53	A_13
ATOM	393	O	SER	43	91.758	39.119	9.834	1.00	17.99	A_13
ATOM	394	N	ASP	44	90.949	39.973	11.771	1.00	10.00	A_13
ATOM	396	CA	ASP	44	92.206	39.908	12.505	1.00	16.90	A_13
ATOM	397	CB	ASP	44	92.057	40.588	13.857	1.00	17.79	A_13
ATOM	398	CG	ASP	44	92.544	42.013	13.839	1.00	15.93	A_13
ATOM	399	OD1	ASP	44	92.605	42.618	14.920	1.00	17.21	A_13
ATOM	400	OD2	ASP	44	92.874	42.533	12.754	1.00	19.50	A_13
ATOM	401	C	ASP	44	92.781	38.523	12.729	1.00	26.12	A_13
ATOM	402	O	ASP	44	93.996	38.362	12.897	1.00	21.21	A_13
ATOM	403	N	VAL	45	91.911	37.523	12.745	1.00	20.89	A_13
ATOM	405	CA	VAL	45	92.353	36.161	12.996	1.00	27.53	A_13
ATOM	406	CB	VAL	45	91.853	35.678	14.381	1.00	16.30	A_13
ATOM	407	CG1	VAL	45	92.557	36.472	15.504	1.00	10.00	A_13
ATOM	408	CG2	VAL	45	90.348	35.857	14.495	1.00	10.86	A_13
ATOM	409	C	VAL	45	91.928	35.187	11.911	1.00	24.33	A_13
ATOM	410	O	VAL	45	91.864	33.978	12.157	1.00	18.84	A_13
ATOM	411	N	THR	46	91.750	35.705	10.694	1.00	16.30	A_13
ATOM	413	CA	THR	46	91.293	34.893	9.574	1.00	14.48	A_13
ATOM	414	CB	THR	46	89.750	34.796	9.662	1.00	22.05	A_13
ATOM	415	OG1	THR	46	89.279	33.609	9.028	1.00	31.53	A_13
ATOM	417	CG2	THR	46	89.112	36.014	9.040	1.00	10.99	A_13
ATOM	418	C	THR	46	91.716	35.575	8.257	1.00	25.10	A_13
ATOM	419	O	THR	46	92.022	36.764	8.256	1.00	17.64	A_13
ATOM	420	N	PRO	47	91.688	34.845	7.114	1.00	15.31	A_13
ATOM	421	CD	PRO	47	91.459	33.398	6.985	1.00	17.94	A_13
ATOM	422	CA	PRO	47	92.069	35.416	5.815	1.00	21.50	A_13
ATOM	423	CB	PRO	47	92.199	34.182	4.911	1.00	17.57	A_13
ATOM	424	CG	PRO	47	92.369	33.041	5.848	1.00	27.45	A_13
ATOM	425	C	PRO	47	90.991	36.348	5.256	1.00	21.44	A_13
ATOM	426	O	PRO	47	91.095	36.788	4.116	1.00	11.08	A_13
ATOM	427	N	LEU	48	89.918	36.567	6.018	1.00	10.00	A_13
ATOM	429	CA	LEU	48	88.826	37.434	5.581	1.00	22.09	A_13
ATOM	430	CB	LEU	48	87.575	37.212	6.432	1.00	15.92	A_13
ATOM	431	CG	LEU	48	86.848	35.867	6.435	1.00	13.58	A_13
ATOM	432	CD1	LEU	48	85.931	35.811	7.654	1.00	25.90	A_13
ATOM	433	CD2	LEU	48	86.073	35.666	5.157	1.00	16.47	A_13
ATOM	434	C	LEU	48	89.156	38.916	5.641	1.00	21.20	A_13
ATOM	435	O	LEU	48	89.936	39.366	6.480	1.00	17.28	A_13
ATOM	436	N	ASN	49	88.569	39.670	4.723	1.00	26.12	A_13
ATOM	438	CA	ASN	49	88.738	41.112	4.717	1.00	26.84	A_13
ATOM	439	CB	ASN	49	89.936	41.569	3.885	1.00	18.29	A_13
ATOM	440	CG	ASN	49	90.010	40.912	2.568	1.00	22.55	A_13
ATOM	441	OD1	ASN	49	90.928	40.131	2.305	1.00	24.41	A_13
ATOM	442	ND2	ASN	49	89.068	41.235	1.693	1.00	46.51	A_13
ATOM	445	C	ASN	49	87.416	41.705	4.259	1.00	12.18	A_13
ATOM	446	O	ASN	49	86.732	41.128	3.400	1.00	20.77	A_13
ATOM	447	N	PHE	50	87.025	42.802	4.900	1.00	21.39	A_13
ATOM	449	CA	PHE	50	85.738	43.439	4.642	1.00	10.00	A_13
ATOM	450	CB	PHE	50	84.914	43.440	5.932	1.00	11.45	A_13
ATOM	451	CG	PHE	50	84.863	42.098	6.629	1.00	10.63	A_13
ATOM	452	CD1	PHE	50	85.886	41.705	7.490	1.00	10.00	A_13
ATOM	453	CD2	PHE	50	83.809	41.216	6.395	1.00	14.63	A_13
ATOM	454	CE1	PHE	50	85.858	40.457	8.097	1.00	26.88	A_13
ATOM	455	CE2	PHE	50	83.773	39.963	7.000	1.00	21.13	A_13
ATOM	456	CZ	PHE	50	84.801	39.581	7.852	1.00	10.30	A_13
ATOM	457	C	PHE	50	85.867	44.842	4.093	1.00	22.56	A_13
ATOM	458	O	PHE	50	86.638	45.644	4.612	1.00	19.33	A_13
ATOM	459	N	THR	51	85.099	45.129	3.044	1.00	21.47	A_13
ATOM	461	CA	THR	51	85.125	46.433	2.371	1.00	24.21	A_13
ATOM	462	CB	THR	51	85.602	46.306	0.895	1.00	15.39	A_13
ATOM	463	OG1	THR	51	86.950	45.811	0.853	1.00	24.33	A_13
ATOM	465	CG2	THR	51	85.551	47.654	0.192	1.00	25.47	A_13
ATOM	466	C	THR	51	83.735	47.048	2.359	1.00	22.17	A_13
ATOM	467	O	THR	51	82.766	46.421	1.912	1.00	20.53	A_13
ATOM	468	N	ARG	52	83.653	48.294	2.797	1.00	16.53	A_13
ATOM	470	CA	ARG	52	82.393	49.004	2.871	1.00	10.00	A_13
ATOM	471	CB	ARG	52	82.490	50.085	3.939	1.00	10.00	A_13
ATOM	472	CG	ARG	52	81.201	50.778	4.259	1.00	12.47	A_13
ATOM	473	CD	ARG	52	81.462	51.879	5.278	1.00	19.61	A_13
ATOM	474	NE	ARG	52	80.371	52.836	5.333	1.00	30.55	A_13
ATOM	476	CZ	ARG	52	80.489	54.074	5.795	1.00	24.06	A_13

ATOM	477	NH1	ARG	52	81.661	54.508	6.257	1.00 21.24	A_13
ATOM	480	NH2	ARG	52	79.421	54.862	5.829	1.00 27.78	A_13
ATOM	483	C	ARG	52	81.980	49.620	1.540	1.00 30.22	A_13
ATOM	484	O	ARG	52	82.782	50.269	0.859	1.00 16.27	A_13
ATOM	485	N	LEU	53	80.730	49.372	1.161	1.00 21.07	A_13
ATOM	487	CA	LEU	53	80.159	49.914	-0.062	1.00 15.73	A_13
ATOM	488	CB	LEU	53	79.435	48.831	-0.868	1.00 11.53	A_13
ATOM	489	CG	LEU	53	80.304	47.770	-1.530	1.00 10.00	A_13
ATOM	490	CD1	LEU	53	79.429	46.790	-2.296	1.00 13.21	A_13
ATOM	491	CD2	LEU	53	81.280	48.443	-2.448	1.00 12.78	A_13
ATOM	492	C	LEU	53	79.149	50.932	0.421	1.00 10.00	A_13
ATOM	493	O	LEU	53	78.463	50.713	1.411	1.00 13.62	A_13
ATOM	494	N	HIS	54	79.043	52.041	-0.283	1.00 15.73	A_13
ATOM	496	CA	HIS	54	78.102	53.065	0.126	1.00 12.47	A_13
ATOM	497	CB	HIS	54	78.765	54.435	0.011	1.00 15.18	A_13
ATOM	498	CG	HIS	54	79.967	54.589	0.884	1.00 21.27	A_13
ATOM	499	CD2	HIS	54	81.207	54.056	0.798	1.00 25.30	A_13
ATOM	500	ND1	HIS	54	79.951	55.338	2.043	1.00 16.48	A_13
ATOM	502	CE1	HIS	54	81.127	55.255	2.633	1.00 21.62	A_13
ATOM	503	NE2	HIS	54	81.910	54.482	1.899	1.00 29.91	A_13
ATOM	505	C	HIS	54	76.796	53.044	-0.664	1.00 15.50	A_13
ATOM	506	O	HIS	54	75.914	53.849	-0.403	1.00 21.80	A_13
ATOM	507	N	ASP	55	76.707	52.178	-1.671	1.00 18.31	A_13
ATOM	509	CA	ASP	55	75.509	52.077	-2.502	1.00 17.23	A_13
ATOM	510	CB	ASP	55	75.645	52.928	-3.773	1.00 19.94	A_13
ATOM	511	CG	ASP	55	75.864	54.393	-3.495	1.00 26.81	A_13
ATOM	512	OD1	ASP	55	75.059	54.991	-2.741	1.00 35.97	A_13
ATOM	513	OD2	ASP	55	76.839	54.948	-4.058	1.00 25.09	A_13
ATOM	514	C	ASP	55	75.343	50.645	-2.970	1.00 21.50	A_13
ATOM	515	O	ASP	55	76.286	49.862	-2.929	1.00 17.45	A_13
ATOM	516	N	GLY	56	74.160	50.337	-3.489	1.00 10.31	A_13
ATOM	518	CA	GLY	56	73.897	49.014	-4.014	1.00 13.67	A_13
ATOM	519	C	GLY	56	73.842	47.869	-3.030	1.00 17.61	A_13
ATOM	520	O	GLY	56	73.683	48.065	-1.825	1.00 12.57	A_13
ATOM	521	N	ILE	57	73.943	46.653	-3.560	1.00 22.27	A_13
ATOM	523	CA	ILE	57	73.895	45.460	-2.737	1.00 11.39	A_13
ATOM	524	CB	ILE	57	72.941	44.391	-3.347	1.00 22.87	A_13
ATOM	525	CG2	ILE	57	73.365	42.995	-2.955	1.00 22.98	A_13
ATOM	526	CG1	ILE	57	71.522	44.582	-2.787	1.00 30.87	A_13
ATOM	527	CD1	ILE	57	71.002	46.022	-2.796	1.00 28.15	A_13
ATOM	528	C	ILE	57	75.289	44.919	-2.446	1.00 22.32	A_13
ATOM	529	O	ILE	57	76.140	44.849	-3.332	1.00 25.00	A_13
ATOM	530	N	ALA	58	75.517	44.631	-1.168	1.00 25.02	A_13
ATOM	532	CA	ALA	58	76.773	44.105	-0.669	1.00 15.45	A_13
ATOM	533	CB	ALA	58	77.366	45.060	0.358	1.00 11.62	A_13
ATOM	534	C	ALA	58	76.438	42.780	-0.006	1.00 12.08	A_13
ATOM	535	O	ALA	58	75.289	42.521	0.307	1.00 13.30	A_13
ATOM	536	N	ASP	59	77.449	41.968	0.247	1.00 14.79	A_13
ATOM	538	CA	ASP	59	77.245	40.675	0.880	1.00 18.50	A_13
ATOM	539	CB	ASP	59	78.608	39.974	1.093	1.00 10.83	A_13
ATOM	540	CG	ASP	59	79.425	39.858	-0.210	1.00 23.35	A_13
ATOM	541	OD1	ASP	59	80.598	40.266	-0.236	1.00 17.98	A_13
ATOM	542	OD2	ASP	59	78.896	39.379	-1.230	1.00 16.89	A_13
ATOM	543	C	ASP	59	76.480	40.806	2.200	1.00 13.69	A_13
ATOM	544	O	ASP	59	75.402	40.227	2.380	1.00 15.93	A_13
ATOM	545	N	ILE	60	77.025	41.596	3.109	1.00 13.15	A_13
ATOM	547	CA	ILE	60	76.422	41.800	4.412	1.00 12.20	A_13
ATOM	548	CB	ILE	60	77.500	41.695	5.508	1.00 12.12	A_13
ATOM	549	CG2	ILE	60	76.921	42.060	6.864	1.00 19.27	A_13
ATOM	550	CG1	ILE	60	78.118	40.287	5.481	1.00 10.00	A_13
ATOM	551	CD1	ILE	60	79.330	40.120	6.360	1.00 10.00	A_13
ATOM	552	C	ILE	60	75.743	43.164	4.456	1.00 17.78	A_13
ATOM	553	O	ILE	60	76.410	44.193	4.478	1.00 18.65	A_13
ATOM	554	N	MET	61	74.416	43.168	4.431	1.00 12.54	A_13
ATOM	556	CA	MET	61	73.640	44.416	4.476	1.00 12.86	A_13
ATOM	557	CB	MET	61	72.385	44.314	3.604	1.00 18.16	A_13
ATOM	558	CG	MET	61	72.634	43.979	2.141	1.00 10.00	A_13
ATOM	559	SD	MET	61	73.374	45.314	1.251	1.00 10.69	A_13
ATOM	560	CE	MET	61	71.836	46.299	0.764	1.00 10.00	A_13
ATOM	561	C	MET	61	73.239	44.666	5.921	1.00 10.15	A_13
ATOM	562	O	MET	61	72.584	43.838	6.547	1.00 18.13	A_13
ATOM	563	N	ILE	62	73.706	45.784	6.456	1.00 15.60	A_13
ATOM	565	CA	ILE	62	73.452	46.170	7.837	1.00 18.55	A_13
ATOM	566	CB	ILE	62	74.723	46.828	8.437	1.00 10.00	A_13
ATOM	567	CG2	ILE	62	74.498	47.163	9.900	1.00 26.36	A_13
ATOM	568	CG1	ILE	62	75.936	45.897	8.302	1.00 11.04	A_13
ATOM	569	CD1	ILE	62	77.228	46.481	8.891	1.00 10.00	A_13

ATOM	570	C	ILE	62	72.289	47.172	7.920	1.00	17.99	A_13
ATOM	571	O	ILE	62	72.335	48.208	7.264	1.00	12.72	A_13
ATOM	572	N	SER	63	71.285	46.896	8.751	1.00	10.00	A_13
ATOM	574	CA	SER	63	70.149	47.803	8.882	1.00	12.52	A_13
ATOM	575	CB	SER	63	69.016	47.364	7.956	1.00	13.06	A_13
ATOM	576	OG	SER	63	68.448	46.146	8.415	1.00	27.90	A_13
ATOM	578	C	SER	63	69.625	47.854	10.314	1.00	13.14	A_13
ATOM	579	O	SER	63	69.869	46.951	11.101	1.00	22.10	A_13
ATOM	580	N	PHE	64	68.919	48.932	10.640	1.00	21.17	A_13
ATOM	582	CA	PHE	64	68.317	49.139	11.954	1.00	22.01	A_13
ATOM	583	CB	PHE	64	68.777	50.468	12.574	1.00	10.98	A_13
ATOM	584	CG	PHE	64	70.189	50.448	13.092	1.00	10.00	A_13
ATOM	585	CD1	PHE	64	70.473	49.885	14.322	1.00	10.00	A_13
ATOM	586	CD2	PHE	64	71.229	51.016	12.357	1.00	16.56	A_13
ATOM	587	CE1	PHE	64	71.777	49.885	14.825	1.00	10.00	A_13
ATOM	588	CE2	PHE	64	72.540	51.025	12.846	1.00	10.00	A_13
ATOM	589	CZ	PHE	64	72.812	50.459	14.081	1.00	18.83	A_13
ATOM	590	C	PHE	64	66.825	49.207	11.675	1.00	22.55	A_13
ATOM	591	O	PHE	64	66.405	49.940	10.779	1.00	19.49	A_13
ATOM	592	N	GLY	65	66.031	48.485	12.453	1.00	13.69	A_13
ATOM	594	CA	GLY	65	64.593	48.491	12.238	1.00	10.70	A_13
ATOM	595	C	GLY	65	63.894	48.138	13.521	1.00	12.62	A_13
ATOM	596	O	GLY	65	64.559	47.777	14.491	1.00	18.29	A_13
ATOM	597	N	ILE	66	62.577	48.309	13.565	1.00	13.69	A_13
ATOM	599	CA	ILE	66	61.803	47.968	14.760	1.00	21.58	A_13
ATOM	600	CB	ILE	66	61.227	49.228	15.503	1.00	30.51	A_13
ATOM	601	CG2	ILE	66	62.351	50.110	16.025	1.00	10.43	A_13
ATOM	602	CG1	ILE	66	60.332	50.062	14.586	1.00	14.56	A_13
ATOM	603	CD1	ILE	66	59.587	51.149	15.333	1.00	16.94	A_13
ATOM	604	C	ILE	66	60.662	47.030	14.361	1.00	10.81	A_13
ATOM	605	O	ILE	66	60.311	46.962	13.188	1.00	10.00	A_13
ATOM	606	N	LYS	67	60.143	46.271	15.330	1.00	10.00	A_13
ATOM	608	CA	LYS	67	59.036	45.327	15.103	1.00	10.23	A_13
ATOM	609	CB	LYS	67	57.689	46.042	15.268	1.00	10.29	A_13
ATOM	610	CG	LYS	67	57.584	46.895	16.510	1.00	14.63	A_13
ATOM	611	CD	LYS	67	57.646	46.056	17.774	1.00	14.94	A_13
ATOM	612	CE	LYS	67	57.382	46.923	18.986	1.00	22.99	A_13
ATOM	613	NZ	LYS	67	57.480	46.174	20.258	1.00	28.27	A_13
ATOM	617	C	LYS	67	59.113	44.633	13.726	1.00	17.91	A_13
ATOM	618	O	LYS	67	60.167	44.106	13.366	1.00	24.16	A_13
ATOM	619	N	GLU	68	58.027	44.690	12.949	1.00	12.72	A_13
ATOM	621	CA	GLU	68	57.960	44.067	11.624	1.00	16.06	A_13
ATOM	622	CB	GLU	68	56.505	44.019	11.128	1.00	26.89	A_13
ATOM	623	CG	GLU	68	55.566	43.258	12.087	1.00	36.97	A_13
ATOM	624	CD	GLU	68	54.217	43.973	12.381	1.00	41.61	A_13
ATOM	625	OE1	GLU	68	53.289	43.921	11.537	1.00	17.31	A_13
ATOM	626	OE2	GLU	68	54.074	44.561	13.485	1.00	26.72	A_13
ATOM	627	C	GLU	68	58.823	44.911	10.705	1.00	22.50	A_13
ATOM	628	O	GLU	68	58.587	46.093	10.532	1.00	20.64	A_13
ATOM	629	N	HIS	69	59.848	44.315	10.120	1.00	16.43	A_13
ATOM	631	CA	HIS	69	60.732	45.102	9.283	1.00	13.69	A_13
ATOM	632	CB	HIS	69	61.930	45.603	10.103	1.00	10.97	A_13
ATOM	633	CG	HIS	69	62.786	44.502	10.643	1.00	24.02	A_13
ATOM	634	CD2	HIS	69	63.873	43.876	10.133	1.00	10.00	A_13
ATOM	635	ND1	HIS	69	62.512	43.876	11.839	1.00	17.68	A_13
ATOM	637	CE1	HIS	69	63.384	42.912	12.041	1.00	12.53	A_13
ATOM	638	NE2	HIS	69	64.228	42.888	11.020	1.00	10.00	A_13
ATOM	639	C	HIS	69	61.214	44.469	7.983	1.00	21.28	A_13
ATOM	640	O	HIS	69	62.314	44.780	7.529	1.00	18.74	A_13
ATOM	641	N	GLY	70	60.451	43.537	7.411	1.00	13.11	A_13
ATOM	643	CA	GLY	70	60.832	42.968	6.127	1.00	10.00	A_13
ATOM	644	C	GLY	70	61.262	41.533	5.936	1.00	10.00	A_13
ATOM	645	O	GLY	70	61.523	41.125	4.794	1.00	15.12	A_13
ATOM	646	N	ASP	71	61.412	40.768	7.012	1.00	19.99	A_13
ATOM	648	CA	ASP	71	61.842	39.381	6.862	1.00	19.99	A_13
ATOM	649	CB	ASP	71	63.332	39.223	7.218	1.00	10.00	A_13
ATOM	650	CG	ASP	71	63.672	39.752	8.592	1.00	23.52	A_13
ATOM	651	OD1	ASP	71	64.846	40.110	8.803	1.00	13.38	A_13
ATOM	652	OD2	ASP	71	62.774	39.812	9.464	1.00	12.94	A_13
ATOM	653	C	ASP	71	60.998	38.377	7.632	1.00	22.07	A_13
ATOM	654	O	ASP	71	61.319	37.190	7.649	1.00	24.45	A_13
ATOM	655	N	PHE	72	59.946	38.865	8.292	1.00	14.15	A_13
ATOM	657	CA	PHE	72	59.040	38.035	9.094	1.00	10.00	A_13
ATOM	658	CB	PHE	72	58.410	36.905	8.272	1.00	10.00	A_13
ATOM	659	CG	PHE	72	57.360	37.387	7.332	1.00	10.00	A_13
ATOM	660	CD1	PHE	72	56.115	37.773	7.815	1.00	23.01	A_13
ATOM	661	CD2	PHE	72	57.624	37.507	5.973	1.00	12.52	A_13

ATOM	662	CE1	PHE	72	55.144	38.290	6.950	1.00	18.99	A_13
ATOM	663	CE2	PHE	72	56.662	38.023	5.091	1.00	13.37	A_13
ATOM	664	CZ	PHE	72	55.420	38.413	5.576	1.00	22.50	A_13
ATOM	665	C	PHE	72	59.634	37.523	10.392	1.00	16.31	A_13
ATOM	666	O	PHE	72	59.111	36.596	11.021	1.00	15.64	A_13
ATOM	667	N	TYR	73	60.737	38.141	10.793	1.00	18.10	A_13
ATOM	669	CA	TYR	73	61.407	37.827	12.046	1.00	14.01	A_13
ATOM	670	CB	TYR	73	62.845	37.331	11.803	1.00	21.08	A_13
ATOM	671	CG	TYR	73	62.915	35.965	11.138	1.00	22.48	A_13
ATOM	672	CD1	TYR	73	63.579	35.788	9.923	1.00	30.23	A_13
ATOM	673	CE1	TYR	73	63.615	34.538	9.291	1.00	24.04	A_13
ATOM	674	CD2	TYR	73	62.288	34.856	11.710	1.00	19.23	A_13
ATOM	675	CE2	TYR	73	62.320	33.606	11.083	1.00	29.35	A_13
ATOM	676	CZ	TYR	73	62.984	33.460	9.875	1.00	12.50	A_13
ATOM	677	OH	TYR	73	63.018	32.246	9.241	1.00	17.89	A_13
ATOM	679	C	TYR	73	61.360	39.203	12.721	1.00	22.00	A_13
ATOM	680	O	TYR	73	62.365	39.919	12.819	1.00	10.93	A_13
ATOM	681	N	PRO	74	60.175	39.570	13.221	1.00	19.94	A_13
ATOM	682	CD	PRO	74	58.969	38.723	13.278	1.00	15.69	A_13
ATOM	683	CA	PRO	74	59.934	40.843	13.886	1.00	16.75	A_13
ATOM	684	CB	PRO	74	58.417	40.836	14.067	1.00	17.27	A_13
ATOM	685	CG	PRO	74	58.131	39.407	14.335	1.00	16.24	A_13
ATOM	686	C	PRO	74	60.640	41.037	15.216	1.00	17.39	A_13
ATOM	687	O	PRO	74	60.779	40.105	16.023	1.00	10.00	A_13
ATOM	688	N	PHE	75	61.098	42.264	15.431	1.00	10.00	A_13
ATOM	690	CA	PHE	75	61.743	42.618	16.675	1.00	16.45	A_13
ATOM	691	CB	PHE	75	62.613	43.865	16.512	1.00	20.71	A_13
ATOM	692	CG	PHE	75	63.931	43.590	15.841	1.00	23.32	A_13
ATOM	693	CD1	PHE	75	64.694	42.482	16.200	1.00	12.03	A_13
ATOM	694	CD2	PHE	75	64.405	44.420	14.842	1.00	22.30	A_13
ATOM	695	CE1	PHE	75	65.905	42.214	15.572	1.00	17.64	A_13
ATOM	696	CE2	PHE	75	65.622	44.148	14.208	1.00	15.43	A_13
ATOM	697	CZ	PHE	75	66.367	43.044	14.576	1.00	10.00	A_13
ATOM	698	C	PHE	75	60.632	42.784	17.707	1.00	25.73	A_13
ATOM	699	O	PHE	75	59.443	42.778	17.370	1.00	18.57	A_13
ATOM	700	N	ASP	76	61.009	43.002	18.952	1.00	20.50	A_13
ATOM	702	CA	ASP	76	60.023	43.049	20.006	1.00	13.89	A_13
ATOM	703	CB	ASP	76	60.241	41.805	20.873	1.00	20.69	A_13
ATOM	704	CG	ASP	76	61.672	41.685	21.378	1.00	22.52	A_13
ATOM	705	OD1	ASP	76	61.947	40.771	22.174	1.00	20.06	A_13
ATOM	706	OD2	ASP	76	62.525	42.506	20.998	1.00	10.69	A_13
ATOM	707	C	ASP	76	59.971	44.277	20.900	1.00	25.20	A_13
ATOM	708	O	ASP	76	59.397	44.207	21.986	1.00	29.52	A_13
ATOM	709	N	GLY	77	60.585	45.379	20.488	1.00	10.00	A_13
ATOM	711	CA	GLY	77	60.575	46.553	21.334	1.00	10.00	A_13
ATOM	712	C	GLY	77	61.769	46.514	22.266	1.00	10.00	A_13
ATOM	713	O	GLY	77	62.735	45.797	21.987	1.00	18.49	A_13
ATOM	714	N	PRO	78	61.785	47.344	23.322	1.00	16.07	A_13
ATOM	715	CD	PRO	78	60.790	48.426	23.505	1.00	15.88	A_13
ATOM	716	CA	PRO	78	62.855	47.439	24.330	1.00	16.23	A_13
ATOM	717	CB	PRO	78	62.261	48.391	25.363	1.00	22.96	A_13
ATOM	718	CG	PRO	78	61.470	49.349	24.501	1.00	22.37	A_13
ATOM	719	C	PRO	78	63.150	46.090	24.969	1.00	25.32	A_13
ATOM	720	O	PRO	78	62.227	45.356	25.272	1.00	20.04	A_13
ATOM	721	N	SER	79	64.432	45.750	25.099	1.00	20.93	A_13
ATOM	723	CA	SER	79	64.878	44.478	25.689	1.00	20.51	A_13
ATOM	724	CB	SER	79	64.364	44.311	27.131	1.00	23.69	A_13
ATOM	725	OG	SER	79	65.028	45.211	28.006	1.00	33.37	A_13
ATOM	727	C	SER	79	64.557	43.248	24.863	1.00	20.39	A_13
ATOM	728	O	SER	79	64.124	43.362	23.708	1.00	17.27	A_13
ATOM	729	N	GLY	80	64.825	42.071	25.415	1.00	13.38	A_13
ATOM	731	CA	GLY	80	64.564	40.850	24.678	1.00	10.11	A_13
ATOM	732	C	GLY	80	65.471	40.808	23.458	1.00	13.15	A_13
ATOM	733	O	GLY	80	66.614	41.251	23.538	1.00	31.80	A_13
ATOM	734	N	LEU	81	64.939	40.393	22.310	1.00	29.05	A_13
ATOM	736	CA	LEU	81	65.720	40.317	21.078	1.00	29.63	A_13
ATOM	737	CB	LEU	81	64.789	40.033	19.905	1.00	19.67	A_13
ATOM	738	CG	LEU	81	65.121	38.872	18.971	1.00	21.79	A_13
ATOM	739	CD1	LEU	81	64.215	38.980	17.773	1.00	23.87	A_13
ATOM	740	CD2	LEU	81	66.590	38.918	18.518	1.00	22.09	A_13
ATOM	741	C	LEU	81	66.442	41.649	20.835	1.00	19.25	A_13
ATOM	742	O	LEU	81	65.808	42.700	20.872	1.00	14.95	A_13
ATOM	743	N	LEU	82	67.760	41.599	20.657	1.00	25.03	A_13
ATOM	745	CA	LEU	82	68.573	42.795	20.421	1.00	27.35	A_13
ATOM	746	CB	LEU	82	69.868	42.747	21.244	1.00	12.74	A_13
ATOM	747	CG	LEU	82	69.802	42.748	22.773	1.00	16.50	A_13
ATOM	748	CD1	LEU	82	68.590	43.520	23.263	1.00	17.99	A_13

ATOM	749	CD2	LEU	82	69.744	41.343	23.279	1.00	13.28	A_13
ATOM	750	C	LEU	82	68.938	42.945	18.949	1.00	24.79	A_13
ATOM	751	O	LEU	82	68.812	44.039	18.363	1.00	14.36	A_13
ATOM	752	N	ALA	83	69.387	41.839	18.359	1.00	21.15	A_13
ATOM	754	CA	ALA	83	69.790	41.819	16.961	1.00	15.64	A_13
ATOM	755	CB	ALA	83	71.180	42.410	16.820	1.00	15.74	A_13
ATOM	756	C	ALA	83	69.806	40.400	16.444	1.00	19.37	A_13
ATOM	757	O	ALA	83	69.864	39.458	17.227	1.00	20.42	A_13
ATOM	758	N	HIS	84	69.746	40.252	15.126	1.00	10.72	A_13
ATOM	760	CA	HIS	84	69.808	38.939	14.502	1.00	20.51	A_13
ATOM	761	CB	HIS	84	68.454	38.185	14.476	1.00	12.34	A_13
ATOM	762	CG	HIS	84	67.361	38.849	13.679	1.00	24.79	A_13
ATOM	763	CD2	HIS	84	67.381	39.489	12.488	1.00	10.00	A_13
ATOM	764	ND1	HIS	84	66.052	38.869	14.104	1.00	13.50	A_13
ATOM	766	CE1	HIS	84	65.307	39.497	13.210	1.00	14.37	A_13
ATOM	767	NE2	HIS	84	66.087	39.886	12.220	1.00	15.00	A_13
ATOM	768	C	HIS	84	70.418	39.088	13.130	1.00	22.78	A_13
ATOM	769	O	HIS	84	70.338	40.162	12.532	1.00	10.00	A_13
ATOM	770	N	ALA	85	71.086	38.027	12.685	1.00	13.43	A_13
ATOM	772	CA	ALA	85	71.746	37.983	11.402	1.00	10.00	A_13
ATOM	773	CB	ALA	85	73.234	38.132	11.596	1.00	10.05	A_13
ATOM	774	C	ALA	85	71.426	36.661	10.721	1.00	17.89	A_13
ATOM	775	O	ALA	85	70.900	35.746	11.346	1.00	19.43	A_13
ATOM	776	N	PHE	86	71.697	36.585	9.425	1.00	13.49	A_13
ATOM	778	CA	PHE	86	71.459	35.372	8.651	1.00	12.49	A_13
ATOM	779	CB	PHE	86	70.739	35.728	7.344	1.00	10.00	A_13
ATOM	780	CG	PHE	86	69.348	36.240	7.529	1.00	19.96	A_13
ATOM	781	CD1	PHE	86	68.252	35.434	7.212	1.00	21.89	A_13
ATOM	782	CD2	PHE	86	69.119	37.530	8.003	1.00	10.63	A_13
ATOM	783	CE1	PHE	86	66.946	35.900	7.364	1.00	16.59	A_13
ATOM	784	CE2	PHE	86	67.829	38.009	8.158	1.00	19.06	A_13
ATOM	785	CZ	PHE	86	66.732	37.194	7.838	1.00	24.79	A_13
ATOM	786	C	PHE	86	72.802	34.721	8.298	1.00	11.05	A_13
ATOM	787	O	PHE	86	73.774	35.435	8.041	1.00	25.56	A_13
ATOM	788	N	PRO	87	72.892	33.375	8.304	1.00	19.41	A_13
ATOM	789	CD	PRO	87	71.876	32.383	8.717	1.00	17.25	A_13
ATOM	790	CA	PRO	87	74.149	32.686	7.956	1.00	29.29	A_13
ATOM	791	CB	PRO	87	73.800	31.198	8.135	1.00	18.88	A_13
ATOM	792	CG	PRO	87	72.329	31.160	7.939	1.00	20.17	A_13
ATOM	793	C	PRO	87	74.562	32.999	6.503	1.00	10.00	A_13
ATOM	794	O	PRO	87	73.728	33.448	5.703	1.00	20.68	A_13
ATOM	795	N	PRO	88	75.814	32.701	6.120	1.00	10.00	A_13
ATOM	796	CD	PRO	88	76.796	31.854	6.831	1.00	19.58	A_13
ATOM	797	CA	PRO	88	76.280	32.977	4.756	1.00	12.43	A_13
ATOM	798	CB	PRO	88	77.600	32.201	4.676	1.00	18.69	A_13
ATOM	799	CG	PRO	88	78.073	32.163	6.098	1.00	18.48	A_13
ATOM	800	C	PRO	88	75.304	32.510	3.672	1.00	24.39	A_13
ATOM	801	O	PRO	88	74.596	31.522	3.854	1.00	16.92	A_13
ATOM	802	N	GLY	89	75.266	33.230	2.560	1.00	10.73	A_13
ATOM	804	CA	GLY	89	74.386	32.868	1.471	1.00	10.00	A_13
ATOM	805	C	GLY	89	73.960	34.127	0.772	1.00	10.94	A_13
ATOM	806	O	GLY	89	74.143	35.218	1.307	1.00	19.86	A_13
ATOM	807	N	PRO	90	73.390	34.019	-0.432	1.00	26.31	A_13
ATOM	808	CD	PRO	90	73.090	32.792	-1.192	1.00	18.46	A_13
ATOM	809	CA	PRO	90	72.960	35.212	-1.163	1.00	25.07	A_13
ATOM	810	CB	PRO	90	72.670	34.651	-2.556	1.00	15.47	A_13
ATOM	811	CG	PRO	90	72.108	33.289	-2.236	1.00	24.63	A_13
ATOM	812	C	PRO	90	71.726	35.879	-0.543	1.00	20.41	A_13
ATOM	813	O	PRO	90	71.176	35.390	0.442	1.00	17.00	A_13
ATOM	814	N	ASN	91	71.303	37.000	-1.125	1.00	18.43	A_13
ATOM	816	CA	ASN	91	70.127	37.721	-0.653	1.00	14.03	A_13
ATOM	817	CB	ASN	91	68.863	36.932	-0.999	1.00	15.26	A_13
ATOM	818	CG	ASN	91	68.860	36.430	-2.439	1.00	36.74	A_13
ATOM	819	OD1	ASN	91	68.497	35.282	-2.701	1.00	29.56	A_13
ATOM	820	ND2	ASN	91	69.265	37.286	-3.376	1.00	27.03	A_13
ATOM	823	C	ASN	91	70.226	37.986	0.849	1.00	24.66	A_13
ATOM	824	O	ASN	91	71.257	38.479	1.313	1.00	17.43	A_13
ATOM	825	N	TYR	92	69.198	37.632	1.622	1.00	17.69	A_13
ATOM	827	CA	TYR	92	69.233	37.876	3.061	1.00	10.17	A_13
ATOM	828	CB	TYR	92	67.942	37.428	3.744	1.00	16.78	A_13
ATOM	829	CG	TYR	92	66.786	38.364	3.523	1.00	26.17	A_13
ATOM	830	CD1	TYR	92	66.015	38.803	4.581	1.00	17.79	A_13
ATOM	831	CE1	TYR	92	64.947	39.678	4.380	1.00	29.60	A_13
ATOM	832	CD2	TYR	92	66.467	38.818	2.250	1.00	25.90	A_13
ATOM	833	CE2	TYR	92	65.406	39.691	2.040	1.00	30.60	A_13
ATOM	834	CZ	TYR	92	64.647	40.117	3.107	1.00	12.31	A_13
ATOM	835	OH	TYR	92	63.575	40.967	2.886	1.00	26.07	A_13

ATOM	837	C	TYR	92	70.427	37.245	3.763	1.00	11.94	A_13
ATOM	838	O	TYR	92	70.752	37.617	4.882	1.00	17.58	A_13
ATOM	839	N	GLY	93	71.095	36.311	3.097	1.00	24.67	A_13
ATOM	841	CA	GLY	93	72.250	35.666	3.691	1.00	18.05	A_13
ATOM	842	C	GLY	93	73.295	36.681	4.116	1.00	10.00	A_13
ATOM	843	O	GLY	93	73.573	37.656	3.391	1.00	10.13	A_13
ATOM	844	N	GLY	94	73.812	36.495	5.328	1.00	12.44	A_13
ATOM	846	CA	GLY	94	74.827	37.372	5.872	1.00	10.00	A_13
ATOM	847	C	GLY	94	74.358	38.694	6.456	1.00	17.29	A_13
ATOM	848	O	GLY	94	75.052	39.271	7.284	1.00	14.53	A_13
ATOM	849	N	ASP	95	73.221	39.206	5.993	1.00	10.00	A_13
ATOM	851	CA	ASP	95	72.689	40.485	6.472	1.00	16.35	A_13
ATOM	852	CB	ASP	95	71.332	40.777	5.814	1.00	10.00	A_13
ATOM	853	CG	ASP	95	71.421	40.904	4.309	1.00	14.54	A_13
ATOM	854	OD1	ASP	95	70.406	41.256	3.673	1.00	11.86	A_13
ATOM	855	OD2	ASP	95	72.502	40.647	3.753	1.00	15.39	A_13
ATOM	856	C	ASP	95	72.548	40.523	7.994	1.00	22.31	A_13
ATOM	857	O	ASP	95	72.279	39.497	8.635	1.00	10.88	A_13
ATOM	858	N	ALA	96	72.703	41.711	8.566	1.00	18.45	A_13
ATOM	860	CA	ALA	96	72.609	41.877	10.011	1.00	15.08	A_13
ATOM	861	CB	ALA	96	73.982	42.244	10.587	1.00	19.20	A_13
ATOM	862	C	ALA	96	71.587	42.961	10.345	1.00	14.91	A_13
ATOM	863	O	ALA	96	71.702	44.092	9.876	1.00	10.00	A_13
ATOM	864	N	HIS	97	70.635	42.646	11.215	1.00	14.01	A_13
ATOM	866	CA	HIS	97	69.599	43.620	11.581	1.00	11.35	A_13
ATOM	867	CB	HIS	97	68.207	43.083	11.203	1.00	20.32	A_13
ATOM	868	CG	HIS	97	68.027	42.786	9.742	1.00	15.00	A_13
ATOM	869	CD2	HIS	97	68.734	43.186	8.654	1.00	10.00	A_13
ATOM	870	ND1	HIS	97	67.014	41.978	9.257	1.00	14.03	A_13
ATOM	871	CE1	HIS	97	67.108	41.895	7.936	1.00	10.00	A_13
ATOM	872	NE2	HIS	97	68.142	42.618	7.552	1.00	17.10	A_13
ATOM	874	C	HIS	97	69.650	43.952	13.078	1.00	13.37	A_13
ATOM	875	O	HIS	97	69.736	43.055	13.908	1.00	13.48	A_13
ATOM	876	N	PHE	98	69.596	45.237	13.423	1.00	21.01	A_13
ATOM	878	CA	PHE	98	69.634	45.668	14.823	1.00	11.27	A_13
ATOM	879	CB	PHE	98	70.817	46.615	15.055	1.00	10.00	A_13
ATOM	880	CG	PHE	98	72.138	46.011	14.703	1.00	20.49	A_13
ATOM	881	CD1	PHE	98	72.984	45.524	15.707	1.00	17.49	A_13
ATOM	882	CD2	PHE	98	72.506	45.853	13.365	1.00	13.51	A_13
ATOM	883	CE1	PHE	98	74.171	44.888	15.382	1.00	20.00	A_13
ATOM	884	CE2	PHE	98	73.693	45.215	13.024	1.00	10.00	A_13
ATOM	885	CZ	PHE	98	74.527	44.728	14.029	1.00	10.00	A_13
ATOM	886	C	PHE	98	68.336	46.336	15.245	1.00	25.38	A_13
ATOM	887	O	PHE	98	67.815	47.218	14.552	1.00	10.00	A_13
ATOM	888	N	ASP	99	67.817	45.924	16.394	1.00	21.68	A_13
ATOM	890	CA	ASP	99	66.567	46.476	16.886	1.00	10.00	A_13
ATOM	891	CB	ASP	99	66.039	45.604	18.010	1.00	10.00	A_13
ATOM	892	CG	ASP	99	64.648	45.998	18.473	1.00	14.00	A_13
ATOM	893	OD1	ASP	99	64.104	45.272	19.329	1.00	15.19	A_13
ATOM	894	OD2	ASP	99	64.089	47.011	18.001	1.00	17.01	A_13
ATOM	895	C	ASP	99	66.817	47.871	17.391	1.00	13.06	A_13
ATOM	896	O	ASP	99	67.528	48.056	18.374	1.00	10.00	A_13
ATOM	897	N	ASP	100	66.203	48.856	16.746	1.00	15.56	A_13
ATOM	899	CA	ASP	100	66.397	50.232	17.177	1.00	18.23	A_13
ATOM	900	CB	ASP	100	66.121	51.228	16.041	1.00	15.05	A_13
ATOM	901	CG	ASP	100	67.275	52.180	15.838	1.00	11.67	A_13
ATOM	902	OD1	ASP	100	67.602	52.516	14.683	1.00	21.07	A_13
ATOM	903	OD2	ASP	100	67.879	52.569	16.860	1.00	14.72	A_13
ATOM	904	C	ASP	100	65.610	50.572	18.445	1.00	10.00	A_13
ATOM	905	O	ASP	100	65.767	51.635	19.009	1.00	17.18	A_13
ATOM	906	N	ASP	101	64.755	49.669	18.895	1.00	14.57	A_13
ATOM	908	CA	ASP	101	64.031	49.924	20.123	1.00	17.59	A_13
ATOM	909	CB	ASP	101	62.769	49.051	20.236	1.00	12.50	A_13
ATOM	910	CG	ASP	101	61.532	49.721	19.606	1.00	17.12	A_13
ATOM	911	OD1	ASP	101	60.599	49.023	19.179	1.00	10.39	A_13
ATOM	912	OD2	ASP	101	61.480	50.962	19.536	1.00	18.09	A_13
ATOM	913	C	ASP	101	64.994	49.766	21.306	1.00	19.33	A_13
ATOM	914	O	ASP	101	64.610	49.972	22.456	1.00	10.00	A_13
ATOM	915	N	GLU	102	66.213	49.301	21.019	1.00	16.15	A_13
ATOM	917	CA	GLU	102	67.267	49.194	22.044	1.00	13.43	A_13
ATOM	918	CB	GLU	102	68.264	48.085	21.720	1.00	18.25	A_13
ATOM	919	CG	GLU	102	67.697	46.704	21.636	1.00	10.00	A_13
ATOM	920	CD	GLU	102	66.650	46.467	22.672	1.00	11.18	A_13
ATOM	921	OE1	GLU	102	66.872	46.746	23.870	1.00	16.09	A_13
ATOM	922	OE2	GLU	102	65.572	46.033	22.271	1.00	26.76	A_13
ATOM	923	C	GLU	102	68.070	50.495	22.007	1.00	11.07	A_13
ATOM	924	O	GLU	102	68.103	51.161	20.971	1.00	13.97	A_13

ATOM	925	N	THR	103	68.774	50.823	23.091	1.00	22.82	A_13
ATOM	927	CA	THR	103	69.606	52.034	23.102	1.00	13.45	A_13
ATOM	928	CB	THR	103	69.571	52.793	24.459	1.00	20.78	A_13
ATOM	929	OG1	THR	103	68.236	53.228	24.745	1.00	10.69	A_13
ATOM	931	CG2	THR	103	70.445	54.046	24.378	1.00	19.45	A_13
ATOM	932	C	THR	103	71.030	51.571	22.822	1.00	12.42	A_13
ATOM	933	O	THR	103	71.639	50.896	23.642	1.00	19.81	A_13
ATOM	934	N	TRP	104	71.525	51.854	21.626	1.00	10.00	A_13
ATOM	936	CA	TRP	104	72.873	51.448	21.248	1.00	13.61	A_13
ATOM	937	CB	TRP	104	72.943	51.221	19.739	1.00	29.21	A_13
ATOM	938	CG	TRP	104	71.970	50.174	19.313	1.00	21.39	A_13
ATOM	939	CD2	TRP	104	72.101	48.760	19.501	1.00	25.13	A_13
ATOM	940	CE2	TRP	104	70.937	48.156	18.964	1.00	28.84	A_13
ATOM	941	CE3	TRP	104	73.088	47.941	20.070	1.00	13.36	A_13
ATOM	942	CD1	TRP	104	70.765	50.372	18.694	1.00	21.59	A_13
ATOM	943	NE1	TRP	104	70.139	49.163	18.484	1.00	19.91	A_13
ATOM	945	CZ2	TRP	104	70.738	46.768	18.977	1.00	10.00	A_13
ATOM	946	CZ3	TRP	104	72.888	46.568	20.084	1.00	14.54	A_13
ATOM	947	CH2	TRP	104	71.720	45.995	19.539	1.00	11.93	A_13
ATOM	948	C	TRP	104	73.912	52.453	21.725	1.00	16.59	A_13
ATOM	949	O	TRP	104	73.707	53.671	21.642	1.00	12.90	A_13
ATOM	950	N	THR	105	75.013	51.949	22.268	1.00	20.85	A_13
ATOM	952	CA	THR	105	76.040	52.831	22.794	1.00	12.38	A_13
ATOM	953	CB	THR	105	75.974	52.890	24.322	1.00	14.39	A_13
ATOM	954	OG1	THR	105	76.345	51.609	24.849	1.00	16.42	A_13
ATOM	956	CG2	THR	105	74.575	53.273	24.797	1.00	12.17	A_13
ATOM	957	C	THR	105	77.437	52.378	22.457	1.00	10.00	A_13
ATOM	958	O	THR	105	77.644	51.261	22.012	1.00	18.98	A_13
ATOM	959	N	SER	106	78.385	53.277	22.704	1.00	26.01	A_13
ATOM	961	CA	SER	106	79.809	53.043	22.502	1.00	17.80	A_13
ATOM	962	CB	SER	106	80.466	54.284	21.888	1.00	20.63	A_13
ATOM	963	OG	SER	106	79.744	54.756	20.763	1.00	38.89	A_13
ATOM	965	C	SER	106	80.435	52.779	23.880	1.00	34.75	A_13
ATOM	966	O	SER	106	81.652	52.884	24.042	1.00	33.01	A_13
ATOM	967	N	SER	107	79.590	52.494	24.875	1.00	25.87	A_13
ATOM	969	CA	SER	107	80.032	52.221	26.240	1.00	19.68	A_13
ATOM	970	CB	SER	107	80.082	53.510	27.061	1.00	23.47	A_13
ATOM	971	OG	SER	107	78.819	54.158	27.096	1.00	33.70	A_13
ATOM	973	C	SER	107	79.100	51.200	26.892	1.00	13.60	A_13
ATOM	974	O	SER	107	78.460	50.418	26.193	1.00	16.40	A_13
ATOM	975	N	SER	108	79.028	51.205	28.221	1.00	17.31	A_13
ATOM	977	CA	SER	108	78.188	50.259	28.949	1.00	20.12	A_13
ATOM	978	CB	SER	108	78.745	50.009	30.364	1.00	22.63	A_13
ATOM	979	OG	SER	108	78.444	51.061	31.271	1.00	27.69	A_13
ATOM	981	C	SER	108	76.702	50.606	29.076	1.00	19.98	A_13
ATOM	982	O	SER	108	75.921	49.785	29.562	1.00	35.96	A_13
ATOM	983	N	LYS	109	76.311	51.820	28.713	1.00	16.24	A_13
ATOM	985	CA	LYS	109	74.907	52.186	28.847	1.00	11.10	A_13
ATOM	986	CB	LYS	109	74.740	53.688	28.690	1.00	12.41	A_13
ATOM	987	CG	LYS	109	73.555	54.239	29.462	1.00	32.67	A_13
ATOM	988	CD	LYS	109	73.353	55.732	29.258	1.00	25.94	A_13
ATOM	989	CE	LYS	109	74.535	56.599	29.749	1.00	25.11	A_13
ATOM	990	NZ	LYS	109	74.225	58.070	29.636	1.00	22.70	A_13
ATOM	994	C	LYS	109	74.138	51.424	27.773	1.00	21.67	A_13
ATOM	995	O	LYS	109	74.667	51.210	26.694	1.00	32.76	A_13
ATOM	996	N	GLY	110	72.932	50.955	28.081	1.00	29.60	A_13
ATOM	998	CA	GLY	110	72.156	50.206	27.096	1.00	10.31	A_13
ATOM	999	C	GLY	110	72.965	49.043	26.542	1.00	20.08	A_13
ATOM	1000	O	GLY	110	73.672	48.362	27.285	1.00	11.17	A_13
ATOM	1001	N	TYR	111	72.924	48.859	25.227	1.00	12.05	A_13
ATOM	1003	CA	TYR	111	73.665	47.791	24.583	1.00	13.45	A_13
ATOM	1004	CB	TYR	111	72.713	46.871	23.806	1.00	21.16	A_13
ATOM	1005	CG	TYR	111	71.776	46.101	24.716	1.00	12.28	A_13
ATOM	1006	CD1	TYR	111	70.455	46.510	24.906	1.00	14.85	A_13
ATOM	1007	CE1	TYR	111	69.618	45.837	25.795	1.00	19.08	A_13
ATOM	1008	CD2	TYR	111	72.232	44.995	25.435	1.00	21.86	A_13
ATOM	1009	CE2	TYR	111	71.405	44.314	26.324	1.00	10.00	A_13
ATOM	1010	CZ	TYR	111	70.101	44.740	26.505	1.00	18.51	A_13
ATOM	1011	OH	TYR	111	69.282	44.077	27.398	1.00	14.32	A_13
ATOM	1013	C	TYR	111	74.779	48.335	23.695	1.00	16.73	A_13
ATOM	1014	O	TYR	111	74.540	49.105	22.764	1.00	11.98	A_13
ATOM	1015	N	ASN	112	76.008	47.930	23.999	1.00	11.80	A_13
ATOM	1017	CA	ASN	112	77.184	48.357	23.240	1.00	16.37	A_13
ATOM	1018	CB	ASN	112	78.453	47.867	23.927	1.00	27.52	A_13
ATOM	1019	CG	ASN	112	79.701	48.460	23.324	1.00	20.16	A_13
ATOM	1020	OD1	ASN	112	80.327	47.861	22.447	1.00	20.99	A_13
ATOM	1021	ND2	ASN	112	80.082	49.640	23.801	1.00	15.12	A_13

ATOM	1024	C	ASN	112	77.137	47.809	21.813	1.00	18.08	A_13
ATOM	1025	O	ASN	112	77.288	46.606	21.592	1.00	12.69	A_13
ATOM	1026	N	LEU	113	76.972	48.700	20.844	1.00	11.15	A_13
ATOM	1028	CA	LEU	113	76.878	48.296	19.461	1.00	10.00	A_13
ATOM	1029	CB	LEU	113	76.718	49.526	18.568	1.00	10.24	A_13
ATOM	1030	CG	LEU	113	76.325	49.262	17.106	1.00	15.67	A_13
ATOM	1031	CD1	LEU	113	75.155	48.296	17.050	1.00	26.54	A_13
ATOM	1032	CD2	LEU	113	75.967	50.555	16.415	1.00	15.60	A_13
ATOM	1033	C	LEU	113	78.037	47.403	18.986	1.00	25.17	A_13
ATOM	1034	O	LEU	113	77.799	46.380	18.336	1.00	17.24	A_13
ATOM	1035	N	PHE	114	79.274	47.759	19.327	1.00	28.89	A_13
ATOM	1037	CA	PHE	114	80.442	46.974	18.910	1.00	19.15	A_13
ATOM	1038	CB	PHE	114	81.753	47.579	19.434	1.00	14.60	A_13
ATOM	1039	CG	PHE	114	82.923	46.627	19.374	1.00	18.53	A_13
ATOM	1040	CD1	PHE	114	83.419	46.175	18.144	1.00	26.13	A_13
ATOM	1041	CD2	PHE	114	83.514	46.162	20.547	1.00	17.22	A_13
ATOM	1042	CE1	PHE	114	84.475	45.271	18.086	1.00	10.43	A_13
ATOM	1043	CE2	PHE	114	84.571	45.259	20.502	1.00	16.51	A_13
ATOM	1044	CZ	PHE	114	85.052	44.815	19.260	1.00	15.54	A_13
ATOM	1045	C	PHE	114	80.359	45.508	19.306	1.00	10.00	A_13
ATOM	1046	O	PHE	114	80.437	44.625	18.445	1.00	33.07	A_13
ATOM	1047	N	LEU	115	80.206	45.249	20.600	1.00	12.18	A_13
ATOM	1049	CA	LEU	115	80.113	43.877	21.103	1.00	10.59	A_13
ATOM	1050	CB	LEU	115	79.874	43.895	22.616	1.00	14.14	A_13
ATOM	1051	CG	LEU	115	81.082	43.937	23.578	1.00	34.39	A_13
ATOM	1052	CD1	LEU	115	82.337	44.354	22.863	1.00	14.93	A_13
ATOM	1053	CD2	LEU	115	80.815	44.836	24.793	1.00	13.42	A_13
ATOM	1054	C	LEU	115	79.019	43.080	20.379	1.00	12.06	A_13
ATOM	1055	O	LEU	115	79.298	42.109	19.675	1.00	13.35	A_13
ATOM	1056	N	VAL	116	77.786	43.558	20.459	1.00	13.11	A_13
ATOM	1058	CA	VAL	116	76.678	42.875	19.814	1.00	12.97	A_13
ATOM	1059	CB	VAL	116	75.343	43.569	20.129	1.00	28.07	A_13
ATOM	1060	CG1	VAL	116	74.200	42.926	19.340	1.00	17.32	A_13
ATOM	1061	CG2	VAL	116	75.074	43.491	21.617	1.00	22.14	A_13
ATOM	1062	C	VAL	116	76.862	42.724	18.313	1.00	10.00	A_13
ATOM	1063	O	VAL	116	76.473	41.716	17.755	1.00	14.68	A_13
ATOM	1064	N	ALA	117	77.481	43.706	17.667	1.00	10.80	A_13
ATOM	1066	CA	ALA	117	77.726	43.662	16.224	1.00	18.28	A_13
ATOM	1067	CB	ALA	117	78.223	45.014	15.727	1.00	14.94	A_13
ATOM	1068	C	ALA	117	78.735	42.579	15.863	1.00	25.24	A_13
ATOM	1069	O	ALA	117	78.562	41.872	14.861	1.00	18.50	A_13
ATOM	1070	N	ALA	118	79.795	42.458	16.665	1.00	24.40	A_13
ATOM	1072	CA	ALA	118	80.829	41.451	16.422	1.00	11.80	A_13
ATOM	1073	CB	ALA	118	81.945	41.590	17.447	1.00	19.28	A_13
ATOM	1074	C	ALA	118	80.178	40.056	16.496	1.00	10.00	A_13
ATOM	1075	O	ALA	118	80.426	39.183	15.660	1.00	10.00	A_13
ATOM	1076	N	HIS	119	79.309	39.875	17.487	1.00	19.01	A_13
ATOM	1078	CA	HIS	119	78.587	38.624	17.674	1.00	14.36	A_13
ATOM	1079	CB	HIS	119	77.725	38.751	18.924	1.00	10.00	A_13
ATOM	1080	CG	HIS	119	76.796	37.602	19.166	1.00	10.00	A_13
ATOM	1081	CD2	HIS	119	75.691	37.187	18.498	1.00	14.94	A_13
ATOM	1082	ND1	HIS	119	76.905	36.783	20.263	1.00	20.37	A_13
ATOM	1084	CE1	HIS	119	75.917	35.909	20.270	1.00	17.53	A_13
ATOM	1085	NE2	HIS	119	75.161	36.134	19.208	1.00	17.55	A_13
ATOM	1086	C	HIS	119	77.741	38.339	16.419	1.00	10.00	A_13
ATOM	1087	O	HIS	119	77.779	37.245	15.856	1.00	10.64	A_13
ATOM	1088	N	GLU	120	77.004	39.343	15.968	1.00	22.95	A_13
ATOM	1090	CA	GLU	120	76.174	39.224	14.775	1.00	23.96	A_13
ATOM	1091	CB	GLU	120	75.429	40.545	14.502	1.00	17.19	A_13
ATOM	1092	CG	GLU	120	74.373	40.889	15.555	1.00	16.14	A_13
ATOM	1093	CD	GLU	120	73.492	39.691	15.929	1.00	10.00	A_13
ATOM	1094	OE1	GLU	120	73.478	39.354	17.122	1.00	17.94	A_13
ATOM	1095	OE2	GLU	120	72.844	39.078	15.047	1.00	17.03	A_13
ATOM	1096	C	GLU	120	76.992	38.832	13.549	1.00	11.45	A_13
ATOM	1097	O	GLU	120	76.594	37.946	12.772	1.00	13.34	A_13
ATOM	1098	N	PHE	121	78.127	39.498	13.353	1.00	10.00	A_13
ATOM	1100	CA	PHE	121	78.959	39.187	12.216	1.00	14.70	A_13
ATOM	1101	CB	PHE	121	80.040	40.245	12.039	1.00	10.00	A_13
ATOM	1102	CG	PHE	121	79.481	41.623	11.792	1.00	21.57	A_13
ATOM	1103	CD1	PHE	121	80.235	42.764	12.069	1.00	16.73	A_13
ATOM	1104	CD2	PHE	121	78.164	41.788	11.331	1.00	13.91	A_13
ATOM	1105	CE1	PHE	121	79.682	44.054	11.891	1.00	11.69	A_13
ATOM	1106	CE2	PHE	121	77.615	43.066	11.152	1.00	18.93	A_13
ATOM	1107	CZ	PHE	121	78.373	44.192	11.436	1.00	10.00	A_13
ATOM	1108	C	PHE	121	79.505	37.756	12.283	1.00	17.14	A_13
ATOM	1109	O	PHE	121	79.642	37.104	11.256	1.00	13.04	A_13
ATOM	1110	N	GLY	122	79.738	37.245	13.490	1.00	16.60	A_13

```
ATOM   1112  CA  GLY   122      80.202  35.872  13.627  1.00 19.45      A_13
ATOM   1113  C   GLY   122      79.162  34.982  12.966  1.00 18.55      A_13
ATOM   1114  O   GLY   122      79.500  33.988  12.306  1.00 10.03      A_13
ATOM   1115  N   HIS   123      77.892  35.361  13.140  1.00 18.22      A_13
ATOM   1117  CA  HIS   123      76.753  34.665  12.525  1.00 16.31      A_13
ATOM   1118  CB  HIS   123      75.424  35.224  13.031  1.00 11.35      A_13
ATOM   1119  CG  HIS   123      75.049  34.768  14.403  1.00 10.33      A_13
ATOM   1120  CD2 HIS   123      74.552  35.454  15.457  1.00 16.64      A_13
ATOM   1121  ND1 HIS   123      75.097  33.450  14.782  1.00 18.04      A_13
ATOM   1123  CE1 HIS   123      74.638  33.332  16.017  1.00 16.66      A_13
ATOM   1124  NE2 HIS   123      74.301  34.533  16.450  1.00 25.32      A_13
ATOM   1125  C   HIS   123      76.771  34.853  10.997  1.00 13.66      A_13
ATOM   1126  O   HIS   123      76.565  33.901  10.246  1.00 10.82      A_13
ATOM   1127  N   SER   124      77.006  36.082  10.539  1.00 13.57      A_13
ATOM   1129  CA  SER   124      77.030  36.368   9.099  1.00 12.03      A_13
ATOM   1130  CB  SER   124      77.311  37.863   8.832  1.00 10.35      A_13
ATOM   1131  OG  SER   124      76.399  38.706   9.510  1.00 14.26      A_13
ATOM   1133  C   SER   124      78.117  35.548   8.422  1.00 21.45      A_13
ATOM   1134  O   SER   124      78.079  35.333   7.210  1.00 10.00      A_13
ATOM   1135  N   LEU   125      79.091  35.108   9.216  1.00 10.00      A_13
ATOM   1137  CA  LEU   125      80.222  34.340   8.707  1.00 19.28      A_13
ATOM   1138  CB  LEU   125      81.521  34.754   9.422  1.00 22.39      A_13
ATOM   1139  CG  LEU   125      81.849  36.258   9.340  1.00 10.00      A_13
ATOM   1140  CD1 LEU   125      83.063  36.622  10.190  1.00 10.00      A_13
ATOM   1141  CD2 LEU   125      82.029  36.651   7.873  1.00 10.00      A_13
ATOM   1142  C   LEU   125      79.986  32.851   8.843  1.00 10.00      A_13
ATOM   1143  O   LEU   125      80.759  32.056   8.329  1.00 23.27      A_13
ATOM   1144  N   GLY   126      78.932  32.477   9.563  1.00 22.87      A_13
ATOM   1146  CA  GLY   126      78.604  31.070   9.720  1.00 17.27      A_13
ATOM   1147  C   GLY   126      78.781  30.464  11.094  1.00 11.71      A_13
ATOM   1148  O   GLY   126      78.784  29.244  11.236  1.00 24.16      A_13
ATOM   1149  N   LEU   127      78.972  31.297  12.105  1.00 18.95      A_13
ATOM   1151  CA  LEU   127      79.152  30.790  13.457  1.00 22.84      A_13
ATOM   1152  CB  LEU   127      80.113  31.693  14.252  1.00 11.92      A_13
ATOM   1153  CG  LEU   127      81.244  30.969  14.983  1.00 18.83      A_13
ATOM   1154  CD1 LEU   127      82.096  30.197  13.979  1.00 16.63      A_13
ATOM   1155  CD2 LEU   127      82.104  31.970  15.760  1.00 22.15      A_13
ATOM   1156  C   LEU   127      77.802  30.699  14.163  1.00 21.02      A_13
ATOM   1157  O   LEU   127      76.996  31.629  14.098  1.00 14.68      A_13
ATOM   1158  N   ASP   128      77.563  29.572  14.828  1.00 18.87      A_13
ATOM   1160  CA  ASP   128      76.336  29.345  15.571  1.00 16.46      A_13
ATOM   1161  CB  ASP   128      75.996  27.855  15.540  1.00 17.60      A_13
ATOM   1162  CG  ASP   128      74.577  27.552  15.996  1.00 23.55      A_13
ATOM   1163  OD1 ASP   128      73.796  28.488  16.258  1.00 10.00      A_13
ATOM   1164  OD2 ASP   128      74.236  26.355  16.087  1.00 32.36      A_13
ATOM   1165  C   ASP   128      76.634  29.803  16.995  1.00 10.00      A_13
ATOM   1166  O   ASP   128      77.650  30.420  17.244  1.00 29.54      A_13
ATOM   1167  N   HIS   129      75.714  29.565  17.912  1.00 10.00      A_13
ATOM   1169  CA  HIS   129      75.910  29.955  19.289  1.00 10.00      A_13
ATOM   1170  CB  HIS   129      74.582  30.033  20.029  1.00 21.30      A_13
ATOM   1171  CG  HIS   129      73.798  31.282  19.761  1.00 24.16      A_13
ATOM   1172  CD2 HIS   129      74.180  32.585  19.725  1.00 10.00      A_13
ATOM   1173  ND1 HIS   129      72.460  31.263  19.476  1.00 21.70      A_13
ATOM   1175  CE1 HIS   129      72.031  32.501  19.271  1.00 10.27      A_13
ATOM   1176  NE2 HIS   129      73.057  33.319  19.407  1.00 14.37      A_13
ATOM   1177  C   HIS   129      76.780  28.947  19.992  1.00 30.04      A_13
ATOM   1178  O   HIS   129      76.624  27.730  19.822  1.00 22.13      A_13
ATOM   1179  N   SER   130      77.628  29.468  20.860  1.00 18.60      A_13
ATOM   1181  CA  SER   130      78.534  28.662  21.636  1.00 10.79      A_13
ATOM   1182  CB  SER   130      79.849  29.435  21.816  1.00 21.31      A_13
ATOM   1183  OG  SER   130      80.782  28.731  22.616  1.00 16.34      A_13
ATOM   1185  C   SER   130      77.898  28.368  22.987  1.00 31.13      A_13
ATOM   1186  O   SER   130      76.962  29.060  23.440  1.00 15.87      A_13
ATOM   1187  N   LYS   131      78.402  27.319  23.619  1.00 13.13      A_13
ATOM   1189  CA  LYS   131      77.924  26.925  24.928  1.00 13.21      A_13
ATOM   1190  CB  LYS   131      77.656  25.414  24.990  1.00 18.85      A_13
ATOM   1191  CG  LYS   131      78.689  24.541  24.303  1.00 32.55      A_13
ATOM   1192  CD  LYS   131      78.547  24.601  22.790  1.00 41.54      A_13
ATOM   1193  CE  LYS   131      79.909  24.672  22.117  1.00 19.64      A_13
ATOM   1194  NZ  LYS   131      80.747  25.799  22.617  1.00 13.47      A_13
ATOM   1198  C   LYS   131      78.922  27.379  25.982  1.00 10.00      A_13
ATOM   1199  O   LYS   131      78.666  27.260  27.185  1.00 13.35      A_13
ATOM   1200  N   ASP   132      80.025  27.968  25.519  1.00 13.47      A_13
ATOM   1202  CA  ASP   132      81.097  28.487  26.375  1.00 10.04      A_13
ATOM   1203  CB  ASP   132      82.376  28.617  25.522  1.00 18.14      A_13
ATOM   1204  CG  ASP   132      83.649  28.821  26.345  1.00 16.54      A_13
ATOM   1205  OD1 ASP   132      84.645  28.132  26.028  1.00 36.08      A_13
```

ATOM	1206	OD2	ASP	132	83.685	29.660	27.276	1.00	15.60	A_13
ATOM	1207	C	ASP	132	80.603	29.875	26.836	1.00	18.74	A_13
ATOM	1208	O	ASP	132	80.559	30.816	26.038	1.00	14.61	A_13
ATOM	1209	N	PRO	133	80.305	30.039	28.142	1.00	15.61	A_13
ATOM	1210	CD	PRO	133	80.617	29.127	29.251	1.00	21.19	A_13
ATOM	1211	CA	PRO	133	79.818	31.320	28.662	1.00	10.00	A_13
ATOM	1212	CB	PRO	133	79.542	31.007	30.135	1.00	10.00	A_13
ATOM	1213	CG	PRO	133	80.633	30.063	30.450	1.00	30.94	A_13
ATOM	1214	C	PRO	133	80.834	32.444	28.511	1.00	22.87	A_13
ATOM	1215	O	PRO	133	80.526	33.574	28.742	1.00	21.65	A_13
ATOM	1216	N	GLY	134	82.070	32.115	28.174	1.00	20.95	A_13
ATOM	1218	CA	GLY	134	83.055	33.167	28.028	1.00	15.22	A_13
ATOM	1219	C	GLY	134	83.182	33.578	26.581	1.00	34.54	A_13
ATOM	1220	O	GLY	134	83.962	34.488	26.252	1.00	18.06	A_13
ATOM	1221	N	ALA	135	82.490	32.846	25.706	1.00	21.09	A_13
ATOM	1223	CA	ALA	135	82.547	33.110	24.263	1.00	27.50	A_13
ATOM	1224	CB	ALA	135	82.131	31.858	23.453	1.00	10.00	A_13
ATOM	1225	C	ALA	135	81.722	34.308	23.814	1.00	21.74	A_13
ATOM	1226	O	ALA	135	80.641	34.556	24.328	1.00	13.84	A_13
ATOM	1227	N	LEU	136	82.220	34.990	22.787	1.00	19.10	A_13
ATOM	1229	CA	LEU	136	81.540	36.140	22.203	1.00	21.65	A_13
ATOM	1230	CB	LEU	136	82.448	36.803	21.161	1.00	10.00	A_13
ATOM	1231	CG	LEU	136	81.964	37.898	20.201	1.00	17.22	A_13
ATOM	1232	CD1	LEU	136	81.250	37.296	19.024	1.00	24.18	A_13
ATOM	1233	CD2	LEU	136	81.113	38.896	20.905	1.00	10.00	A_13
ATOM	1234	C	LEU	136	80.250	35.632	21.558	1.00	19.32	A_13
ATOM	1235	O	LEU	136	79.266	36.359	21.458	1.00	26.20	A_13
ATOM	1236	N	MET	137	80.297	34.409	21.029	1.00	10.00	A_13
ATOM	1238	CA	MET	137	79.123	33.791	20.423	1.00	10.02	A_13
ATOM	1239	CB	MET	137	79.507	32.691	19.428	1.00	15.14	A_13
ATOM	1240	CG	MET	137	80.181	33.223	18.169	1.00	16.42	A_13
ATOM	1241	SD	MET	137	79.366	34.665	17.397	1.00	10.65	A_13
ATOM	1242	CE	MET	137	77.848	34.005	16.975	1.00	10.87	A_13
ATOM	1243	C	MET	137	78.122	33.256	21.447	1.00	12.70	A_13
ATOM	1244	O	MET	137	77.187	32.539	21.087	1.00	10.00	A_13
ATOM	1245	N	PHE	138	78.295	33.627	22.713	1.00	18.70	A_13
ATOM	1247	CA	PHE	138	77.370	33.196	23.759	1.00	24.08	A_13
ATOM	1248	CB	PHE	138	77.954	33.448	25.159	1.00	24.15	A_13
ATOM	1249	CG	PHE	138	77.306	32.617	26.240	1.00	29.38	A_13
ATOM	1250	CD1	PHE	138	76.694	33.222	27.336	1.00	27.07	A_13
ATOM	1251	CD2	PHE	138	77.253	31.226	26.123	1.00	21.37	A_13
ATOM	1252	CE1	PHE	138	76.033	32.455	28.289	1.00	30.35	A_13
ATOM	1253	CE2	PHE	138	76.599	30.458	27.065	1.00	19.58	A_13
ATOM	1254	CZ	PHE	138	75.986	31.070	28.154	1.00	17.69	A_13
ATOM	1255	C	PHE	138	76.074	33.992	23.513	1.00	14.20	A_13
ATOM	1256	O	PHE	138	76.115	35.105	23.014	1.00	10.27	A_13
ATOM	1257	N	PRO	139	74.899	33.366	23.730	1.00	13.04	A_13
ATOM	1258	CD	PRO	139	74.664	31.975	24.131	1.00	11.17	A_13
ATOM	1259	CA	PRO	139	73.619	34.043	23.504	1.00	18.27	A_13
ATOM	1260	CB	PRO	139	72.625	32.875	23.384	1.00	14.33	A_13
ATOM	1261	CG	PRO	139	73.474	31.634	23.305	1.00	24.22	A_13
ATOM	1262	C	PRO	139	73.162	35.018	24.584	1.00	16.51	A_13
ATOM	1263	O	PRO	139	72.023	35.467	24.535	1.00	24.45	A_13
ATOM	1264	N	ILE	140	74.034	35.375	25.524	1.00	23.16	A_13
ATOM	1266	CA	ILE	140	73.652	36.290	26.604	1.00	25.00	A_13
ATOM	1267	CB	ILE	140	73.688	35.559	27.966	1.00	12.10	A_13
ATOM	1268	CG2	ILE	140	73.336	36.519	29.085	1.00	12.62	A_13
ATOM	1269	CG1	ILE	140	72.738	34.341	27.904	1.00	22.67	A_13
ATOM	1270	CD1	ILE	140	72.827	33.353	29.073	1.00	27.73	A_13
ATOM	1271	C	ILE	140	74.584	37.489	26.621	1.00	30.64	A_13
ATOM	1272	O	ILE	140	75.778	37.317	26.682	1.00	23.16	A_13
ATOM	1273	N	TYR	141	74.033	38.694	26.532	1.00	21.05	A_13
ATOM	1275	CA	TYR	141	74.851	39.901	26.528	1.00	20.10	A_13
ATOM	1276	CB	TYR	141	74.017	41.122	26.129	1.00	17.66	A_13
ATOM	1277	CG	TYR	141	74.784	42.433	26.103	1.00	22.24	A_13
ATOM	1278	CD1	TYR	141	74.711	43.318	27.171	1.00	18.07	A_13
ATOM	1279	CE1	TYR	141	75.386	44.527	27.144	1.00	19.84	A_13
ATOM	1280	CD2	TYR	141	75.565	42.790	24.999	1.00	18.08	A_13
ATOM	1281	CE2	TYR	141	76.244	44.008	24.961	1.00	10.00	A_13
ATOM	1282	CZ	TYR	141	76.149	44.867	26.038	1.00	25.17	A_13
ATOM	1283	OH	TYR	141	76.814	46.070	26.043	1.00	30.78	A_13
ATOM	1285	C	TYR	141	75.533	40.169	27.852	1.00	19.61	A_13
ATOM	1286	O	TYR	141	74.910	40.146	28.913	1.00	16.08	A_13
ATOM	1287	N	THR	142	76.817	40.476	27.772	1.00	26.26	A_13
ATOM	1289	CA	THR	142	77.612	40.788	28.944	1.00	24.52	A_13
ATOM	1290	CB	THR	142	78.498	39.568	29.362	1.00	10.00	A_13
ATOM	1291	OG1	THR	142	77.664	38.587	29.981	1.00	37.30	A_13

```
ATOM   1293  CG2 THR   142      79.543  39.961  30.390  1.00 14.88      A_13
ATOM   1294  C   THR   142      78.467  41.976  28.580  1.00 25.46      A_13
ATOM   1295  O   THR   142      78.980  42.058  27.464  1.00 10.00      A_13
ATOM   1296  N   TYR   143      78.575  42.947  29.476  1.00 20.23      A_13
ATOM   1298  CA  TYR   143      79.412  44.079  29.133  1.00 32.69      A_13
ATOM   1299  CB  TYR   143      79.024  45.363  29.854  1.00 35.01      A_13
ATOM   1300  CG  TYR   143      79.834  46.531  29.347  1.00 16.01      A_13
ATOM   1301  CD1 TYR   143      79.776  46.910  27.998  1.00 12.56      A_13
ATOM   1302  CE1 TYR   143      80.554  47.961  27.510  1.00 19.23      A_13
ATOM   1303  CD2 TYR   143      80.690  47.230  30.196  1.00 19.43      A_13
ATOM   1304  CE2 TYR   143      81.478  48.287  29.719  1.00 15.52      A_13
ATOM   1305  CZ  TYR   143      81.403  48.643  28.376  1.00 12.56      A_13
ATOM   1306  OH  TYR   143      82.193  49.654  27.892  1.00 18.85      A_13
ATOM   1308  C   TYR   143      80.871  43.754  29.382  1.00 25.10      A_13
ATOM   1309  O   TYR   143      81.373  43.846  30.503  1.00 28.90      A_13
ATOM   1310  N   THR   144      81.539  43.375  28.303  1.00 35.25      A_13
ATOM   1312  CA  THR   144      82.946  43.029  28.336  1.00 38.86      A_13
ATOM   1313  CB  THR   144      83.158  41.568  27.873  1.00 23.22      A_13
ATOM   1314  OG1 THR   144      82.129  41.219  26.934  1.00 35.22      A_13
ATOM   1316  CG2 THR   144      83.105  40.616  29.082  1.00 17.53      A_13
ATOM   1317  C   THR   144      83.720  44.017  27.488  1.00 21.63      A_13
ATOM   1318  O   THR   144      84.434  43.651  26.556  1.00 37.44      A_13
ATOM   1319  N   GLY   145      83.504  45.288  27.798  1.00 14.47      A_13
ATOM   1321  CA  GLY   145      84.200  46.375  27.131  1.00 24.39      A_13
ATOM   1322  C   GLY   145      84.119  46.536  25.628  1.00 41.65      A_13
ATOM   1323  O   GLY   145      84.053  45.565  24.877  1.00 42.39      A_13
ATOM   1324  N   LYS   146      84.122  47.792  25.195  1.00 33.04      A_13
ATOM   1326  CA  LYS   146      84.059  48.103  23.778  1.00 29.29      A_13
ATOM   1327  CB  LYS   146      83.260  49.392  23.539  1.00 26.47      A_13
ATOM   1328  CG  LYS   146      83.087  49.721  22.059  1.00 33.24      A_13
ATOM   1329  CD  LYS   146      82.812  51.194  21.833  1.00 13.70      A_13
ATOM   1330  CE  LYS   146      82.620  51.497  20.343  1.00 18.35      A_13
ATOM   1331  NZ  LYS   146      83.766  51.122  19.477  1.00 30.66      A_13
ATOM   1335  C   LYS   146      85.491  48.297  23.308  1.00 41.61      A_13
ATOM   1336  O   LYS   146      86.028  49.412  23.382  1.00 46.44      A_13
ATOM   1337  N   SER   147      86.130  47.206  22.898  1.00 34.67      A_13
ATOM   1339  CA  SER   147      87.509  47.258  22.416  1.00 30.76      A_13
ATOM   1340  CB  SER   147      87.624  48.258  21.249  1.00 24.56      A_13
ATOM   1341  OG  SER   147      86.638  48.002  20.257  1.00 31.81      A_13
ATOM   1343  C   SER   147      88.464  47.626  23.567  1.00 33.60      A_13
ATOM   1344  O   SER   147      88.789  48.806  23.789  1.00 39.96      A_13
ATOM   1345  N   HIS   148      88.862  46.611  24.331  1.00 36.71      A_13
ATOM   1347  CA  HIS   148      89.778  46.769  25.467  1.00 34.40      A_13
ATOM   1348  CB  HIS   148      89.307  47.862  26.438  1.00 26.40      A_13
ATOM   1349  CG  HIS   148      90.251  49.022  26.537  1.00 39.11      A_13
ATOM   1350  CD2 HIS   148      90.929  49.542  27.588  1.00 30.52      A_13
ATOM   1351  ND1 HIS   148      90.635  49.767  25.437  1.00 37.71      A_13
ATOM   1353  CE1 HIS   148      91.511  50.681  25.807  1.00 29.04      A_13
ATOM   1354  NE2 HIS   148      91.707  50.567  27.110  1.00 29.03      A_13
ATOM   1356  C   HIS   148      89.949  45.436  26.190  1.00 39.41      A_13
ATOM   1357  O   HIS   148      90.134  45.373  27.411  1.00 35.01      A_13
ATOM   1358  N   PHE   149      89.840  44.386  25.383  1.00 25.35      A_13
ATOM   1360  CA  PHE   149      89.996  42.966  25.721  1.00 30.54      A_13
ATOM   1361  CB  PHE   149      88.788  42.423  26.495  1.00 33.34      A_13
ATOM   1362  CG  PHE   149      88.951  42.440  27.996  1.00 31.37      A_13
ATOM   1363  CD1 PHE   149      89.387  41.302  28.673  1.00 30.46      A_13
ATOM   1364  CD2 PHE   149      88.624  43.575  28.740  1.00 40.67      A_13
ATOM   1365  CE1 PHE   149      89.492  41.293  30.075  1.00 18.92      A_13
ATOM   1366  CE2 PHE   149      88.728  43.574  30.136  1.00 23.23      A_13
ATOM   1367  CZ  PHE   149      89.161  42.430  30.803  1.00 17.03      A_13
ATOM   1368  C   PHE   149      90.026  42.366  24.295  1.00 41.76      A_13
ATOM   1369  O   PHE   149      89.967  43.119  23.307  1.00 40.43      A_13
ATOM   1370  N   MET   150      90.132  41.050  24.142  1.00 31.30      A_13
ATOM   1372  CA  MET   150      90.152  40.531  22.779  1.00 20.65      A_13
ATOM   1373  CB  MET   150      91.588  40.195  22.352  1.00 28.29      A_13
ATOM   1374  CG  MET   150      92.494  41.436  22.188  1.00 34.71      A_13
ATOM   1375  SD  MET   150      91.750  42.780  21.185  1.00 67.91      A_13
ATOM   1376  CE  MET   150      92.512  42.498  19.518  1.00 22.43      A_13
ATOM   1377  C   MET   150      89.201  39.370  22.497  1.00 21.51      A_13
ATOM   1378  O   MET   150      88.498  38.901  23.391  1.00 25.37      A_13
ATOM   1379  N   LEU   151      89.159  38.938  21.240  1.00 13.78      A_13
ATOM   1381  CA  LEU   151      88.313  37.825  20.834  1.00 14.73      A_13
ATOM   1382  CB  LEU   151      88.435  37.589  19.321  1.00 15.49      A_13
ATOM   1383  CG  LEU   151      87.535  36.511  18.691  1.00 27.05      A_13
ATOM   1384  CD1 LEU   151      86.070  36.915  18.847  1.00 10.98      A_13
ATOM   1385  CD2 LEU   151      87.879  36.310  17.208  1.00 15.73      A_13
ATOM   1386  C   LEU   151      88.732  36.563  21.600  1.00 25.01      A_13
```

ATOM	1387	O	LEU	151	89.912	36.178	21.589	1.00	17.37	A_13
ATOM	1388	N	PRO	152	87.777	35.927	22.306	1.00	10.37	A_13
ATOM	1389	CD	PRO	152	86.425	36.450	22.575	1.00	15.35	A_13
ATOM	1390	CA	PRO	152	88.030	34.712	23.087	1.00	11.49	A_13
ATOM	1391	CB	PRO	152	86.658	34.412	23.702	1.00	15.98	A_13
ATOM	1392	CG	PRO	152	86.083	35.789	23.898	1.00	27.60	A_13
ATOM	1393	C	PRO	152	88.533	33.553	22.230	1.00	18.06	A_13
ATOM	1394	O	PRO	152	88.160	33.430	21.063	1.00	16.21	A_13
ATOM	1395	N	ASP	153	89.350	32.696	22.836	1.00	15.86	A_13
ATOM	1397	CA	ASP	153	89.933	31.526	22.185	1.00	20.25	A_13
ATOM	1398	CB	ASP	153	90.632	30.630	23.227	1.00	18.17	A_13
ATOM	1399	CG	ASP	153	91.843	31.301	23.908	1.00	24.01	A_13
ATOM	1400	OD1	ASP	153	92.517	32.159	23.284	1.00	14.96	A_13
ATOM	1401	OD2	ASP	153	92.131	30.937	25.077	1.00	20.20	A_13
ATOM	1402	C	ASP	153	88.887	30.678	21.452	1.00	24.64	A_13
ATOM	1403	O	ASP	153	89.113	30.221	20.330	1.00	13.51	A_13
ATOM	1404	N	ASP	154	87.757	30.453	22.114	1.00	24.11	A_13
ATOM	1406	CA	ASP	154	86.664	29.657	21.577	1.00	19.19	A_13
ATOM	1407	CB	ASP	154	85.527	29.632	22.587	1.00	18.27	A_13
ATOM	1408	CG	ASP	154	84.406	28.751	22.161	1.00	24.26	A_13
ATOM	1409	OD1	ASP	154	83.314	29.291	21.950	1.00	20.97	A_13
ATOM	1410	OD2	ASP	154	84.609	27.530	22.031	1.00	20.32	A_13
ATOM	1411	C	ASP	154	86.162	30.170	20.229	1.00	18.99	A_13
ATOM	1412	O	ASP	154	86.043	29.408	19.277	1.00	22.56	A_13
ATOM	1413	N	ASP	155	85.873	31.465	20.158	1.00	16.11	A_13
ATOM	1415	CA	ASP	155	85.407	32.078	18.917	1.00	25.30	A_13
ATOM	1416	CB	ASP	155	85.011	33.527	19.158	1.00	13.32	A_13
ATOM	1417	CG	ASP	155	83.975	33.655	20.249	1.00	11.19	A_13
ATOM	1418	OD1	ASP	155	84.347	34.136	21.332	1.00	12.26	A_13
ATOM	1419	OD2	ASP	155	82.810	33.255	20.029	1.00	10.00	A_13
ATOM	1420	C	ASP	155	86.461	31.992	17.828	1.00	13.98	A_13
ATOM	1421	O	ASP	155	86.141	31.656	16.687	1.00	14.08	A_13
ATOM	1422	N	VAL	156	87.713	32.310	18.160	1.00	16.49	A_13
ATOM	1424	CA	VAL	156	88.771	32.201	17.159	1.00	27.34	A_13
ATOM	1425	CB	VAL	156	90.145	32.826	17.625	1.00	23.59	A_13
ATOM	1426	CG1	VAL	156	90.327	32.750	19.119	1.00	13.94	A_13
ATOM	1427	CG2	VAL	156	91.312	32.153	16.919	1.00	21.70	A_13
ATOM	1428	C	VAL	156	88.874	30.738	16.657	1.00	16.95	A_13
ATOM	1429	O	VAL	156	88.946	30.506	15.448	1.00	13.79	A_13
ATOM	1430	N	GLN	157	88.762	29.763	17.561	1.00	19.45	A_13
ATOM	1432	CA	GLN	157	88.796	28.352	17.154	1.00	30.53	A_13
ATOM	1433	CB	GLN	157	88.579	27.422	18.353	1.00	23.08	A_13
ATOM	1434	CG	GLN	157	89.633	27.521	19.452	1.00	24.83	A_13
ATOM	1435	CD	GLN	157	90.950	26.872	19.089	1.00	20.26	A_13
ATOM	1436	OE1	GLN	157	91.743	27.422	18.316	1.00	25.80	A_13
ATOM	1437	NE2	GLN	157	91.204	25.702	19.673	1.00	38.67	A_13
ATOM	1440	C	GLN	157	87.667	28.136	16.148	1.00	14.16	A_13
ATOM	1441	O	GLN	157	87.869	27.541	15.096	1.00	14.11	A_13
ATOM	1442	N	GLY	158	86.505	28.709	16.437	1.00	19.16	A_13
ATOM	1444	CA	GLY	158	85.361	28.584	15.551	1.00	12.79	A_13
ATOM	1445	C	GLY	158	85.510	29.144	14.143	1.00	24.46	A_13
ATOM	1446	O	GLY	158	85.181	28.449	13.177	1.00	18.77	A_13
ATOM	1447	N	ILE	159	85.936	30.403	13.989	1.00	22.41	A_13
ATOM	1449	CA	ILE	159	86.091	30.946	12.628	1.00	31.18	A_13
ATOM	1450	CB	ILE	159	86.300	32.508	12.532	1.00	23.53	A_13
ATOM	1451	CG2	ILE	159	84.991	33.203	12.177	1.00	17.28	A_13
ATOM	1452	CG1	ILE	159	87.022	33.063	13.758	1.00	15.28	A_13
ATOM	1453	CD1	ILE	159	88.507	32.949	13.707	1.00	14.71	A_13
ATOM	1454	C	ILE	159	87.226	30.280	11.875	1.00	10.56	A_13
ATOM	1455	O	ILE	159	87.167	30.139	10.653	1.00	18.79	A_13
ATOM	1456	N	GLN	160	88.287	29.927	12.590	1.00	20.71	A_13
ATOM	1458	CA	GLN	160	89.411	29.294	11.943	1.00	10.00	A_13
ATOM	1459	CB	GLN	160	90.640	29.274	12.855	1.00	10.00	A_13
ATOM	1460	CG	GLN	160	91.114	30.690	13.182	1.00	13.93	A_13
ATOM	1461	CD	GLN	160	92.402	30.754	13.981	1.00	25.61	A_13
ATOM	1462	OE1	GLN	160	92.814	29.786	14.629	1.00	19.40	A_13
ATOM	1463	NE2	GLN	160	93.042	31.915	13.950	1.00	24.78	A_13
ATOM	1466	C	GLN	160	89.000	27.917	11.477	1.00	10.00	A_13
ATOM	1467	O	GLN	160	89.458	27.481	10.432	1.00	21.73	A_13
ATOM	1468	N	SER	161	88.068	27.268	12.186	1.00	10.00	A_13
ATOM	1470	CA	SER	161	87.610	25.946	11.760	1.00	11.63	A_13
ATOM	1471	CB	SER	161	86.688	25.292	12.800	1.00	18.40	A_13
ATOM	1472	OG	SER	161	85.365	25.795	12.759	1.00	15.44	A_13
ATOM	1474	C	SER	161	86.913	26.048	10.396	1.00	26.18	A_13
ATOM	1475	O	SER	161	86.839	25.065	9.654	1.00	13.96	A_13
ATOM	1476	N	LEU	162	86.428	27.247	10.070	1.00	19.36	A_13
ATOM	1478	CA	LEU	162	85.749	27.493	8.808	1.00	17.21	A_13

```
ATOM   1479  CB  LEU   162      84.584  28.477   9.007  1.00 14.37      A_13
ATOM   1480  CG  LEU   162      83.489  28.144  10.021  1.00 31.09      A_13
ATOM   1481  CD1 LEU   162      82.596  29.351  10.217  1.00 14.96      A_13
ATOM   1482  CD2 LEU   162      82.672  26.949   9.548  1.00 23.87      A_13
ATOM   1483  C   LEU   162      86.654  28.080   7.744  1.00 11.98      A_13
ATOM   1484  O   LEU   162      86.596  27.680   6.584  1.00 15.25      A_13
ATOM   1485  N   TYR   163      87.459  29.063   8.135  1.00 26.64      A_13
ATOM   1487  CA  TYR   163      88.320  29.796   7.204  1.00 18.28      A_13
ATOM   1488  CB  TYR   163      87.977  31.289   7.277  1.00 26.89      A_13
ATOM   1489  CG  TYR   163      86.519  31.600   7.039  1.00 18.80      A_13
ATOM   1490  CD1 TYR   163      86.027  31.744   5.749  1.00 10.00      A_13
ATOM   1491  CE1 TYR   163      84.680  31.936   5.515  1.00 12.83      A_13
ATOM   1492  CD2 TYR   163      85.622  31.672   8.099  1.00 16.58      A_13
ATOM   1493  CE2 TYR   163      84.266  31.867   7.873  1.00 12.32      A_13
ATOM   1494  CZ  TYR   163      83.807  31.991   6.576  1.00 11.77      A_13
ATOM   1495  OH  TYR   163      82.472  32.141   6.331  1.00 21.93      A_13
ATOM   1497  C   TYR   163      89.818  29.669   7.397  1.00 15.67      A_13
ATOM   1498  O   TYR   163      90.590  30.089   6.526  1.00 18.92      A_13
ATOM   1499  N   GLY   164      90.225  29.096   8.525  1.00 18.34      A_13
ATOM   1501  CA  GLY   164      91.636  28.966   8.826  1.00 10.61      A_13
ATOM   1502  C   GLY   164      92.149  30.215   9.525  1.00 15.63      A_13
ATOM   1503  O   GLY   164      91.334  31.139   9.775  1.00 21.42      A_13
ATOM   1504  OT  GLY   164      93.353  30.250   9.858  1.00 21.99      A_13
ATOM   3009  ZN  ZN    166      73.275  35.223  18.371  1.00 27.40      AION
ATOM   3010  ZN  ZN    167      65.511  41.122  10.564  1.00 27.86      AION
ATOM   3011  CA  CA    168      64.285  44.152  21.635  1.00 11.76      AION
ATOM   3012  CA  CA    165      73.319  39.377   1.854  1.00 40.73      AION
ATOM   3017  C5  WAY   169      67.400  35.999  20.267  1.00 38.86      A693
ATOM   3018  CF1 WAY   169      66.626  35.606  19.161  1.00 30.96      A693
ATOM   3019  CH  WAY   169      67.199  35.400  17.901  1.00 41.17      A693
ATOM   3020  C2  WAY   169      68.561  35.623  17.728  1.00 36.26      A693
ATOM   3021  C3  WAY   169      69.339  36.039  18.811  1.00 35.73      A693
ATOM   3022  C4  WAY   169      68.807  36.216  20.078  1.00 33.71      A693
ATOM   3023  N20 WAY   169      69.699  36.617  21.141  1.00 33.16      A693
ATOM   3024  CD  WAY   169      70.137  35.640  22.189  1.00 29.78      A693
ATOM   3025  C23 WAY   169      68.986  34.739  22.685  1.00 25.69      A693
ATOM   3026  C28 WAY   169      68.187  35.088  23.798  1.00 31.72      A693
ATOM   3027  C27 WAY   169      67.141  34.238  24.205  1.00 33.61      A693
ATOM   3028  CM  WAY   169      66.921  33.061  23.490  1.00 32.16      A693
ATOM   3029  N25 WAY   169      67.703  32.748  22.426  1.00 42.39      A693
ATOM   3030  C24 WAY   169      68.709  33.546  22.016  1.00 27.88      A693
ATOM   3031  S21 WAY   169      69.757  38.213  21.577  1.00 24.43      A693
ATOM   3032  C16 WAY   169      71.513  38.570  21.438  1.00 29.69      A693
ATOM   3033  C21 WAY   169      72.032  39.163  20.269  1.00 19.32      A693
ATOM   3034  C20 WAY   169      73.400  39.453  20.169  1.00 11.82      A693
ATOM   3035  C19 WAY   169      74.267  39.156  21.241  1.00 19.50      A693
ATOM   3036  C18 WAY   169      73.748  38.564  22.402  1.00 11.88      A693
ATOM   3037  C17 WAY   169      72.382  38.272  22.507  1.00 26.57      A693
ATOM   3038  O33 WAY   169      75.623  39.445  21.141  1.00 16.99      A693
ATOM   3039  C36 WAY   169      76.504  39.509  22.271  1.00 12.69      A693
ATOM   3040  O15 WAY   169      69.030  39.032  20.657  1.00 13.98      A693
ATOM   3041  O14 WAY   169      69.419  38.338  22.942  1.00 22.94      A693
ATOM   3042  C7  WAY   169      70.780  36.256  18.621  1.00 30.48      A693
ATOM   3043  N9  WAY   169      71.192  36.946  17.553  1.00 10.00      A693
ATOM   3044  O10 WAY   169      72.581  37.127  17.426  1.00 38.25      A693
ATOM   3045  O8  WAY   169      71.614  35.847  19.414  1.00 39.46      A693
ATOM   3046  C29 WAY   169      66.584  36.175  21.566  1.00 46.13      A693
ATOM   1505  CB  THR     7      40.443  57.305   5.225  1.00 21.20      B_13
ATOM   1506  OG1 THR     7      39.149  56.999   5.762  1.00 25.31      B_13
ATOM   1508  CG2 THR     7      41.017  56.087   4.541  1.00 23.15      B_13
ATOM   1509  C   THR     7      40.920  59.113   6.901  1.00 32.45      B_13
ATOM   1510  O   THR     7      41.453  59.582   7.908  1.00 36.97      B_13
ATOM   1513  N   THR     7      41.386  56.786   7.488  1.00 34.12      B_13
ATOM   1515  CA  THR     7      41.371  57.761   6.365  1.00 26.16      B_13
ATOM   1516  N   LEU     8      39.907  59.694   6.265  1.00 23.60      B_13
ATOM   1518  CA  LEU     8      39.387  60.984   6.649  1.00 22.66      B_13
ATOM   1519  CB  LEU     8      38.113  60.848   7.503  1.00 21.78      B_13
ATOM   1520  CG  LEU     8      36.860  61.484   6.863  1.00 27.13      B_13
ATOM   1521  CD1 LEU     8      36.996  63.016   6.705  1.00 19.05      B_13
ATOM   1522  CD2 LEU     8      36.622  60.854   5.510  1.00 19.23      B_13
ATOM   1523  C   LEU     8      40.432  61.896   7.298  1.00 27.16      B_13
ATOM   1524  O   LEU     8      41.077  62.667   6.597  1.00 46.24      B_13
ATOM   1525  N   LYS     9      40.615  61.804   8.618  1.00 27.84      B_13
ATOM   1527  CA  LYS     9      41.572  62.674   9.306  1.00 15.20      B_13
ATOM   1528  CB  LYS     9      41.147  64.143   9.148  1.00 32.32      B_13
ATOM   1529  CG  LYS     9      39.663  64.342   8.853  1.00 29.47      B_13
ATOM   1530  CD  LYS     9      38.788  64.243  10.084  1.00 28.34      B_13
```

ATOM	1531	CE	LYS	9	38.830	65.556	10.842	1.00	18.48	B_13
ATOM	1532	NZ	LYS	9	38.732	66.725	9.888	1.00	33.19	B_13
ATOM	1536	C	LYS	9	41.809	62.384	10.780	1.00	20.69	B_13
ATOM	1537	O	LYS	9	41.268	61.428	11.334	1.00	25.62	B_13
ATOM	1538	N	TRP	10	42.654	63.208	11.390	1.00	12.09	B_13
ATOM	1540	CA	TRP	10	42.988	63.112	12.813	1.00	21.78	B_13
ATOM	1541	CB	TRP	10	44.403	63.660	13.048	1.00	23.03	B_13
ATOM	1542	CG	TRP	10	45.499	62.890	12.349	1.00	27.60	B_13
ATOM	1543	CD2	TRP	10	46.077	61.650	12.762	1.00	27.28	B_13
ATOM	1544	CE2	TRP	10	47.071	61.302	11.829	1.00	22.11	B_13
ATOM	1545	CE3	TRP	10	45.859	60.781	13.847	1.00	11.66	B_13
ATOM	1546	CD1	TRP	10	46.153	63.247	11.198	1.00	21.84	B_13
ATOM	1547	NE1	TRP	10	47.094	62.305	10.873	1.00	10.00	B_13
ATOM	1549	CZ2	TRP	10	47.847	60.143	11.929	1.00	25.24	B_13
ATOM	1550	CZ3	TRP	10	46.632	59.622	13.951	1.00	22.71	B_13
ATOM	1551	CH2	TRP	10	47.611	59.317	12.999	1.00	15.23	B_13
ATOM	1552	C	TRP	10	41.987	63.915	13.679	1.00	30.88	B_13
ATOM	1553	O	TRP	10	41.673	65.062	13.359	1.00	32.03	B_13
ATOM	1554	N	SER	11	41.495	63.316	14.765	1.00	35.64	B_13
ATOM	1556	CA	SER	11	40.548	63.981	15.665	1.00	30.37	B_13
ATOM	1557	CB	SER	11	39.498	62.995	16.176	1.00	31.03	B_13
ATOM	1558	OG	SER	11	38.485	62.815	15.202	1.00	41.11	B_13
ATOM	1560	C	SER	11	41.206	64.691	16.840	1.00	20.70	B_13
ATOM	1561	O	SER	11	40.558	65.002	17.838	1.00	36.52	B_13
ATOM	1562	N	LYS	12	42.504	64.910	16.731	1.00	23.56	B_13
ATOM	1564	CA	LYS	12	43.257	65.607	17.756	1.00	15.00	B_13
ATOM	1565	CB	LYS	12	43.991	64.631	18.688	1.00	18.58	B_13
ATOM	1566	CG	LYS	12	44.658	63.452	18.010	1.00	15.94	B_13
ATOM	1567	CD	LYS	12	45.456	62.589	19.007	1.00	23.03	B_13
ATOM	1568	CE	LYS	12	44.593	61.715	19.933	1.00	27.10	B_13
ATOM	1569	NZ	LYS	12	44.075	62.402	21.157	1.00	34.75	B_13
ATOM	1573	C	LYS	12	44.200	66.453	16.914	1.00	25.03	B_13
ATOM	1574	O	LYS	12	44.567	66.039	15.808	1.00	25.20	B_13
ATOM	1575	N	MET	13	44.536	67.647	17.401	1.00	18.44	B_13
ATOM	1577	CA	MET	13	45.377	68.582	16.663	1.00	24.63	B_13
ATOM	1578	CB	MET	13	44.864	70.015	16.880	1.00	13.15	B_13
ATOM	1579	CG	MET	13	43.421	70.253	16.419	1.00	21.56	B_13
ATOM	1580	SD	MET	13	43.167	70.131	14.616	1.00	31.39	B_13
ATOM	1581	CE	MET	13	41.433	69.678	14.474	1.00	24.70	B_13
ATOM	1582	C	MET	13	46.850	68.468	17.034	1.00	11.65	B_13
ATOM	1583	O	MET	13	47.728	68.815	16.247	1.00	14.33	B_13
ATOM	1584	N	ASN	14	47.103	67.985	18.242	1.00	16.99	B_13
ATOM	1586	CA	ASN	14	48.448	67.793	18.760	1.00	24.42	B_13
ATOM	1587	CB	ASN	14	48.437	68.006	20.268	1.00	17.84	B_13
ATOM	1588	CG	ASN	14	47.896	69.356	20.633	1.00	35.10	B_13
ATOM	1589	OD1	ASN	14	48.614	70.346	20.560	1.00	34.88	B_13
ATOM	1590	ND2	ASN	14	46.610	69.424	20.955	1.00	32.98	B_13
ATOM	1593	C	ASN	14	48.831	66.364	18.421	1.00	22.70	B_13
ATOM	1594	O	ASN	14	48.278	65.405	18.976	1.00	26.03	B_13
ATOM	1595	N	LEU	15	49.706	66.228	17.432	1.00	18.07	B_13
ATOM	1597	CA	LEU	15	50.144	64.912	16.969	1.00	29.36	B_13
ATOM	1598	CB	LEU	15	49.878	64.775	15.466	1.00	24.35	B_13
ATOM	1599	CG	LEU	15	48.380	64.762	15.162	1.00	19.51	B_13
ATOM	1600	CD1	LEU	15	48.079	65.469	13.852	1.00	27.59	B_13
ATOM	1601	CD2	LEU	15	47.902	63.326	15.163	1.00	19.66	B_13
ATOM	1602	C	LEU	15	51.613	64.704	17.257	1.00	28.48	B_13
ATOM	1603	O	LEU	15	52.341	65.657	17.552	1.00	22.28	B_13
ATOM	1604	N	THR	16	52.044	63.453	17.198	1.00	12.77	B_13
ATOM	1606	CA	THR	16	53.433	63.158	17.446	1.00	16.59	B_13
ATOM	1607	CB	THR	16	53.607	62.243	18.682	1.00	24.73	B_13
ATOM	1608	OG1	THR	16	52.912	61.005	18.481	1.00	12.79	B_13
ATOM	1610	CG2	THR	16	53.059	62.933	19.924	1.00	25.34	B_13
ATOM	1611	C	THR	16	54.038	62.515	16.214	1.00	21.94	B_13
ATOM	1612	O	THR	16	53.315	62.116	15.297	1.00	19.60	B_13
ATOM	1613	N	TYR	17	55.365	62.453	16.184	1.00	18.25	B_13
ATOM	1615	CA	TYR	17	56.092	61.810	15.097	1.00	19.54	B_13
ATOM	1616	CB	TYR	17	56.300	62.753	13.910	1.00	16.87	B_13
ATOM	1617	CG	TYR	17	57.277	63.892	14.116	1.00	27.90	B_13
ATOM	1618	CD1	TYR	17	56.839	65.135	14.587	1.00	13.93	B_13
ATOM	1619	CE1	TYR	17	57.700	66.221	14.652	1.00	17.08	B_13
ATOM	1620	CD2	TYR	17	58.613	63.764	13.723	1.00	14.99	B_13
ATOM	1621	CE2	TYR	17	59.479	64.841	13.777	1.00	25.98	B_13
ATOM	1622	CZ	TYR	17	59.017	66.075	14.242	1.00	33.12	B_13
ATOM	1623	OH	TYR	17	59.866	67.163	14.276	1.00	23.31	B_13
ATOM	1625	C	TYR	17	57.417	61.318	15.650	1.00	18.57	B_13
ATOM	1626	O	TYR	17	57.895	61.827	16.668	1.00	26.60	B_13
ATOM	1627	N	ARG	18	57.973	60.286	15.030	1.00	13.01	B_13

ATOM	1629	CA	ARG	18	59.245	59.750	15.492	1.00	18.74	B_13
ATOM	1630	CB	ARG	18	59.033	58.589	16.473	1.00	11.96	B_13
ATOM	1631	CG	ARG	18	60.320	57.911	16.970	1.00	15.06	B_13
ATOM	1632	CD	ARG	18	60.012	56.596	17.690	1.00	11.72	B_13
ATOM	1633	NE	ARG	18	61.165	55.689	17.752	1.00	10.00	B_13
ATOM	1635	CZ	ARG	18	61.134	54.428	18.181	1.00	24.87	B_13
ATOM	1636	NH1	ARG	18	60.004	53.882	18.614	1.00	13.34	B_13
ATOM	1639	NH2	ARG	18	62.247	53.703	18.169	1.00	20.03	B_13
ATOM	1642	C	ARG	18	60.076	59.309	14.307	1.00	13.14	B_13
ATOM	1643	O	ARG	18	59.598	58.588	13.434	1.00	14.10	B_13
ATOM	1644	N	ILE	19	61.304	59.813	14.252	1.00	15.55	B_13
ATOM	1646	CA	ILE	19	62.238	59.476	13.193	1.00	10.41	B_13
ATOM	1647	CB	ILE	19	63.307	60.603	13.054	1.00	17.20	B_13
ATOM	1648	CG2	ILE	19	64.273	60.307	11.903	1.00	16.57	B_13
ATOM	1649	CG1	ILE	19	62.613	61.952	12.836	1.00	15.47	B_13
ATOM	1650	CD1	ILE	19	63.543	63.110	12.783	1.00	14.99	B_13
ATOM	1651	C	ILE	19	62.870	58.166	13.673	1.00	10.00	B_13
ATOM	1652	O	ILE	19	63.829	58.179	14.434	1.00	10.00	B_13
ATOM	1653	N	VAL	20	62.289	57.037	13.276	1.00	17.84	B_13
ATOM	1655	CA	VAL	20	62.785	55.716	13.696	1.00	16.43	B_13
ATOM	1656	CB	VAL	20	61.911	54.570	13.138	1.00	13.17	B_13
ATOM	1657	CG1	VAL	20	62.519	53.208	13.493	1.00	10.00	B_13
ATOM	1658	CG2	VAL	20	60.521	54.673	13.698	1.00	10.00	B_13
ATOM	1659	C	VAL	20	64.268	55.449	13.387	1.00	16.02	B_13
ATOM	1660	O	VAL	20	65.001	54.909	14.218	1.00	21.07	B_13
ATOM	1661	N	ASN	21	64.698	55.762	12.177	1.00	10.00	B_13
ATOM	1663	CA	ASN	21	66.098	55.571	11.830	1.00	22.13	B_13
ATOM	1664	CB	ASN	21	66.392	54.128	11.386	1.00	19.75	B_13
ATOM	1665	CG	ASN	21	65.549	53.673	10.212	1.00	17.63	B_13
ATOM	1666	OD1	ASN	21	65.329	52.477	10.042	1.00	31.82	B_13
ATOM	1667	ND2	ASN	21	65.109	54.602	9.375	1.00	11.42	B_13
ATOM	1670	C	ASN	21	66.504	56.645	10.821	1.00	10.14	B_13
ATOM	1671	O	ASN	21	65.639	57.377	10.340	1.00	11.74	B_13
ATOM	1672	N	TYR	22	67.787	56.759	10.498	1.00	12.25	B_13
ATOM	1674	CA	TYR	22	68.233	57.829	9.602	1.00	12.46	B_13
ATOM	1675	CB	TYR	22	69.136	58.800	10.383	1.00	23.15	B_13
ATOM	1676	CG	TYR	22	68.461	59.584	11.492	1.00	21.95	B_13
ATOM	1677	CD1	TYR	22	68.221	60.945	11.348	1.00	22.29	B_13
ATOM	1678	CE1	TYR	22	67.625	61.678	12.347	1.00	10.00	B_13
ATOM	1679	CD2	TYR	22	68.077	58.974	12.687	1.00	13.42	B_13
ATOM	1680	CE2	TYR	22	67.471	59.710	13.693	1.00	14.69	B_13
ATOM	1681	CZ	TYR	22	67.254	61.064	13.505	1.00	12.89	B_13
ATOM	1682	OH	TYR	22	66.660	61.829	14.466	1.00	16.56	B_13
ATOM	1684	C	TYR	22	68.988	57.395	8.359	1.00	11.62	B_13
ATOM	1685	O	TYR	22	69.793	56.478	8.407	1.00	16.23	B_13
ATOM	1686	N	THR	23	68.792	58.111	7.261	1.00	10.39	B_13
ATOM	1688	CA	THR	23	69.503	57.800	6.024	1.00	20.36	B_13
ATOM	1689	CB	THR	23	68.909	58.582	4.829	1.00	16.21	B_13
ATOM	1690	OG1	THR	23	69.801	58.512	3.706	1.00	19.72	B_13
ATOM	1692	CG2	THR	23	68.663	60.039	5.206	1.00	16.62	B_13
ATOM	1693	C	THR	23	70.990	58.153	6.163	1.00	17.35	B_13
ATOM	1694	O	THR	23	71.377	58.958	7.024	1.00	13.88	B_13
ATOM	1695	N	PRO	24	71.852	57.503	5.364	1.00	15.86	B_13
ATOM	1696	CD	PRO	24	71.625	56.247	4.629	1.00	17.29	B_13
ATOM	1697	CA	PRO	24	73.287	57.796	5.436	1.00	15.96	B_13
ATOM	1698	CB	PRO	24	73.920	56.570	4.763	1.00	10.00	B_13
ATOM	1699	CG	PRO	24	72.891	55.504	4.905	1.00	15.15	B_13
ATOM	1700	C	PRO	24	73.635	59.069	4.668	1.00	27.08	B_13
ATOM	1701	O	PRO	24	74.698	59.656	4.869	1.00	19.47	B_13
ATOM	1702	N	ASP	25	72.728	59.489	3.794	1.00	16.99	B_13
ATOM	1704	CA	ASP	25	72.927	60.663	2.958	1.00	10.00	B_13
ATOM	1705	CB	ASP	25	71.792	60.758	1.953	1.00	11.53	B_13
ATOM	1706	CG	ASP	25	71.665	59.521	1.105	1.00	33.88	B_13
ATOM	1707	OD1	ASP	25	70.570	59.311	0.556	1.00	22.66	B_13
ATOM	1708	OD2	ASP	25	72.653	58.762	0.980	1.00	29.59	B_13
ATOM	1709	C	ASP	25	73.068	62.011	3.642	1.00	23.36	B_13
ATOM	1710	O	ASP	25	73.694	62.916	3.093	1.00	20.32	B_13
ATOM	1711	N	MET	26	72.480	62.158	4.826	1.00	18.44	B_13
ATOM	1713	CA	MET	26	72.510	63.432	5.537	1.00	13.83	B_13
ATOM	1714	CB	MET	26	71.154	64.151	5.368	1.00	10.00	B_13
ATOM	1715	CG	MET	26	70.782	64.491	3.913	1.00	28.32	B_13
ATOM	1716	SD	MET	26	69.016	64.786	3.599	1.00	12.18	B_13
ATOM	1717	CE	MET	26	68.395	63.255	3.887	1.00	37.25	B_13
ATOM	1718	C	MET	26	72.827	63.238	7.024	1.00	28.80	B_13
ATOM	1719	O	MET	26	72.839	62.107	7.533	1.00	20.90	B_13
ATOM	1720	N	THR	27	73.157	64.333	7.696	1.00	11.47	B_13
ATOM	1722	CA	THR	27	73.456	64.292	9.121	1.00	13.94	B_13

ATOM	1723	CB	THR	27	74.117	65.605	9.602	1.00	33.46	B_13
ATOM	1724	OG1	THR	27	73.209	66.702	9.415	1.00	10.00	B_13
ATOM	1726	CG2	THR	27	75.405	65.863	8.818	1.00	16.30	B_13
ATOM	1727	C	THR	27	72.135	64.113	9.861	1.00	10.67	B_13
ATOM	1728	O	THR	27	71.072	64.343	9.281	1.00	16.26	B_13
ATOM	1729	N	HIS	28	72.193	63.691	11.124	1.00	18.13	B_13
ATOM	1731	CA	HIS	28	70.986	63.514	11.915	1.00	10.00	B_13
ATOM	1732	CB	HIS	28	71.322	63.033	13.333	1.00	10.00	B_13
ATOM	1733	CG	HIS	28	71.793	61.608	13.401	1.00	22.65	B_13
ATOM	1734	CD2	HIS	28	72.893	61.003	12.889	1.00	22.73	B_13
ATOM	1735	ND1	HIS	28	71.103	60.627	14.080	1.00	19.90	B_13
ATOM	1737	CE1	HIS	28	71.755	59.481	13.985	1.00	16.52	B_13
ATOM	1738	NE2	HIS	28	72.843	59.681	13.268	1.00	20.38	B_13
ATOM	1740	C	HIS	28	70.281	64.870	11.957	1.00	29.38	B_13
ATOM	1741	O	HIS	28	69.074	64.941	11.742	1.00	17.20	B_13
ATOM	1742	N	SER	29	71.056	65.944	12.153	1.00	23.96	B_13
ATOM	1744	CA	SER	29	70.533	67.322	12.192	1.00	15.01	B_13
ATOM	1745	CB	SER	29	71.661	68.334	12.438	1.00	14.05	B_13
ATOM	1746	OG	SER	29	72.117	68.303	13.770	1.00	18.32	B_13
ATOM	1748	C	SER	29	69.808	67.729	10.909	1.00	10.95	B_13
ATOM	1749	O	SER	29	68.732	68.314	10.971	1.00	24.24	B_13
ATOM	1750	N	GLU	30	70.415	67.449	9.757	1.00	10.96	B_13
ATOM	1752	CA	GLU	30	69.820	67.786	8.470	1.00	10.00	B_13
ATOM	1753	CB	GLU	30	70.715	67.330	7.309	1.00	10.12	B_13
ATOM	1754	CG	GLU	30	71.967	68.143	7.042	1.00	22.31	B_13
ATOM	1755	CD	GLU	30	72.823	67.529	5.930	1.00	10.15	B_13
ATOM	1756	OE1	GLU	30	72.533	67.753	4.749	1.00	31.98	B_13
ATOM	1757	OE2	GLU	30	73.796	66.817	6.223	1.00	29.59	B_13
ATOM	1758	C	GLU	30	68.481	67.073	8.336	1.00	20.17	B_13
ATOM	1759	O	GLU	30	67.493	67.685	7.943	1.00	14.31	B_13
ATOM	1760	N	VAL	31	68.451	65.777	8.665	1.00	19.26	B_13
ATOM	1762	CA	VAL	31	67.228	64.989	8.536	1.00	14.22	B_13
ATOM	1763	CB	VAL	31	67.472	63.487	8.716	1.00	17.05	B_13
ATOM	1764	CG1	VAL	31	66.144	62.749	8.791	1.00	28.55	B_13
ATOM	1765	CG2	VAL	31	68.269	62.935	7.548	1.00	10.54	B_13
ATOM	1766	C	VAL	31	66.138	65.458	9.477	1.00	12.36	B_13
ATOM	1767	O	VAL	31	64.963	65.488	9.093	1.00	12.83	B_13
ATOM	1768	N	GLU	32	66.530	65.805	10.703	1.00	20.46	B_13
ATOM	1770	CA	GLU	32	65.596	66.306	11.710	1.00	16.04	B_13
ATOM	1771	CB	GLU	32	66.269	66.365	13.094	1.00	14.71	B_13
ATOM	1772	CG	GLU	32	66.512	64.985	13.741	1.00	23.30	B_13
ATOM	1773	CD	GLU	32	67.724	64.930	14.700	1.00	21.41	B_13
ATOM	1774	OE1	GLU	32	68.229	63.823	15.003	1.00	15.79	B_13
ATOM	1775	OE2	GLU	32	68.183	65.985	15.157	1.00	13.71	B_13
ATOM	1776	C	GLU	32	65.125	67.697	11.257	1.00	27.19	B_13
ATOM	1777	O	GLU	32	63.951	68.042	11.383	1.00	19.82	B_13
ATOM	1778	N	LYS	33	66.021	68.461	10.636	1.00	12.52	B_13
ATOM	1780	CA	LYS	33	65.663	69.786	10.171	1.00	13.00	B_13
ATOM	1781	CB	LYS	33	66.889	70.592	9.762	1.00	22.63	B_13
ATOM	1782	CG	LYS	33	66.581	72.054	9.560	1.00	18.24	B_13
ATOM	1783	CD	LYS	33	65.604	72.545	10.630	1.00	29.21	B_13
ATOM	1784	CE	LYS	33	66.185	72.429	12.048	1.00	41.79	B_13
ATOM	1785	NZ	LYS	33	65.181	71.939	13.054	1.00	20.17	B_13
ATOM	1789	C	LYS	33	64.698	69.686	9.023	1.00	10.62	B_13
ATOM	1790	O	LYS	33	63.734	70.437	8.971	1.00	22.94	B_13
ATOM	1791	N	ALA	34	64.915	68.707	8.150	1.00	10.00	B_13
ATOM	1793	CA	ALA	34	64.050	68.475	7.000	1.00	11.94	B_13
ATOM	1794	CB	ALA	34	64.611	67.374	6.100	1.00	10.00	B_13
ATOM	1795	C	ALA	34	62.640	68.115	7.423	1.00	10.00	B_13
ATOM	1796	O	ALA	34	61.675	68.650	6.878	1.00	15.32	B_13
ATOM	1797	N	PHE	35	62.510	67.208	8.387	1.00	21.32	B_13
ATOM	1799	CA	PHE	35	61.187	66.789	8.852	1.00	18.32	B_13
ATOM	1800	CB	PHE	35	61.267	65.451	9.614	1.00	25.48	B_13
ATOM	1801	CG	PHE	35	61.620	64.260	8.735	1.00	14.33	B_13
ATOM	1802	CD1	PHE	35	61.149	64.171	7.427	1.00	17.91	B_13
ATOM	1803	CD2	PHE	35	62.436	63.240	9.217	1.00	18.05	B_13
ATOM	1804	CE1	PHE	35	61.486	63.086	6.610	1.00	18.49	B_13
ATOM	1805	CE2	PHE	35	62.778	62.158	8.413	1.00	15.01	B_13
ATOM	1806	CZ	PHE	35	62.301	62.081	7.103	1.00	10.00	B_13
ATOM	1807	C	PHE	35	60.428	67.862	9.658	1.00	18.68	B_13
ATOM	1808	O	PHE	35	59.202	67.971	9.556	1.00	17.05	B_13
ATOM	1809	N	LYS	36	61.160	68.664	10.425	1.00	16.30	B_13
ATOM	1811	CA	LYS	36	60.579	69.749	11.229	1.00	19.34	B_13
ATOM	1812	CB	LYS	36	61.676	70.420	12.052	1.00	24.61	B_13
ATOM	1813	CG	LYS	36	61.200	71.293	13.191	1.00	18.38	B_13
ATOM	1814	CD	LYS	36	62.408	71.795	13.962	1.00	19.34	B_13
ATOM	1815	CE	LYS	36	62.067	72.267	15.356	1.00	21.80	B_13

```
ATOM   1816  NZ  LYS    36      63.299  72.615  16.118  1.00 27.76       B_13
ATOM   1820  C   LYS    36      59.924  70.770  10.301  1.00 10.19       B_13
ATOM   1821  O   LYS    36      58.788  71.183  10.528  1.00 14.95       B_13
ATOM   1822  N   LYS    37      60.630  71.134   9.233  1.00 15.89       B_13
ATOM   1824  CA  LYS    37      60.126  72.076   8.230  1.00 19.95       B_13
ATOM   1825  CB  LYS    37      61.202  72.386   7.189  1.00 10.00       B_13
ATOM   1826  CG  LYS    37      62.209  73.439   7.569  1.00 13.18       B_13
ATOM   1827  CD  LYS    37      62.869  73.966   6.311  1.00 28.86       B_13
ATOM   1828  CE  LYS    37      61.825  74.460   5.281  1.00 31.44       B_13
ATOM   1829  NZ  LYS    37      60.878  75.512   5.772  1.00 26.23       B_13
ATOM   1833  C   LYS    37      58.939  71.482   7.472  1.00 25.64       B_13
ATOM   1834  O   LYS    37      57.968  72.177   7.161  1.00 24.39       B_13
ATOM   1835  N   ALA    38      59.060  70.205   7.128  1.00 17.12       B_13
ATOM   1837  CA  ALA    38      58.031  69.493   6.381  1.00 16.06       B_13
ATOM   1838  CB  ALA    38      58.459  68.038   6.154  1.00 12.19       B_13
ATOM   1839  C   ALA    38      56.692  69.557   7.094  1.00 11.12       B_13
ATOM   1840  O   ALA    38      55.648  69.736   6.458  1.00 31.10       B_13
ATOM   1841  N   PHE    39      56.732  69.393   8.417  1.00 21.01       B_13
ATOM   1843  CA  PHE    39      55.540  69.446   9.257  1.00 10.85       B_13
ATOM   1844  CB  PHE    39      55.841  68.833  10.639  1.00 14.45       B_13
ATOM   1845  CG  PHE    39      55.851  67.325  10.659  1.00 21.88       B_13
ATOM   1846  CD1 PHE    39      57.016  66.625  10.954  1.00 16.88       B_13
ATOM   1847  CD2 PHE    39      54.675  66.599  10.442  1.00 22.14       B_13
ATOM   1848  CE1 PHE    39      57.010  65.223  11.037  1.00 17.95       B_13
ATOM   1849  CE2 PHE    39      54.655  65.190  10.522  1.00 17.22       B_13
ATOM   1850  CZ  PHE    39      55.823  64.503  10.823  1.00 13.51       B_13
ATOM   1851  C   PHE    39      55.044  70.898   9.426  1.00 19.98       B_13
ATOM   1852  O   PHE    39      53.839  71.160   9.393  1.00 14.30       B_13
ATOM   1853  N   LYS    40      55.981  71.826   9.611  1.00 20.03       B_13
ATOM   1855  CA  LYS    40      55.681  73.245   9.795  1.00 18.64       B_13
ATOM   1856  CB  LYS    40      56.989  74.011  10.020  1.00 19.28       B_13
ATOM   1857  CG  LYS    40      57.064  75.392   9.440  1.00 26.34       B_13
ATOM   1858  CD  LYS    40      58.288  76.093   9.974  1.00 18.46       B_13
ATOM   1859  CE  LYS    40      58.021  76.673  11.339  1.00 20.86       B_13
ATOM   1860  NZ  LYS    40      57.053  77.814  11.232  1.00 27.28       B_13
ATOM   1864  C   LYS    40      54.899  73.790   8.612  1.00 20.57       B_13
ATOM   1865  O   LYS    40      54.034  74.654   8.756  1.00 22.54       B_13
ATOM   1866  N   VAL    41      55.216  73.251   7.445  1.00 17.15       B_13
ATOM   1868  CA  VAL    41      54.565  73.576   6.184  1.00 19.19       B_13
ATOM   1869  CB  VAL    41      55.095  72.566   5.086  1.00 17.28       B_13
ATOM   1870  CG1 VAL    41      53.987  72.064   4.160  1.00 10.00       B_13
ATOM   1871  CG2 VAL    41      56.224  73.191   4.293  1.00 19.38       B_13
ATOM   1872  C   VAL    41      53.026  73.472   6.354  1.00 20.38       B_13
ATOM   1873  O   VAL    41      52.268  74.280   5.810  1.00 28.57       B_13
ATOM   1874  N   TRP    42      52.587  72.511   7.163  1.00 23.10       B_13
ATOM   1876  CA  TRP    42      51.166  72.265   7.403  1.00 19.29       B_13
ATOM   1877  CB  TRP    42      50.912  70.757   7.487  1.00 22.19       B_13
ATOM   1878  CG  TRP    42      51.437  70.007   6.313  1.00 19.32       B_13
ATOM   1879  CD2 TRP    42      50.836  69.909   5.015  1.00 31.02       B_13
ATOM   1880  CE2 TRP    42      51.659  69.067   4.238  1.00 22.49       B_13
ATOM   1881  CE3 TRP    42      49.677  70.448   4.434  1.00 15.54       B_13
ATOM   1882  CD1 TRP    42      52.571  69.251   6.269  1.00 14.04       B_13
ATOM   1883  NE1 TRP    42      52.710  68.681   5.027  1.00 13.55       B_13
ATOM   1885  CZ2 TRP    42      51.360  68.752   2.912  1.00 18.87       B_13
ATOM   1886  CZ3 TRP    42      49.383  70.132   3.116  1.00 13.33       B_13
ATOM   1887  CH2 TRP    42      50.219  69.294   2.370  1.00 20.30       B_13
ATOM   1888  C   TRP    42      50.617  72.926   8.660  1.00 24.68       B_13
ATOM   1889  O   TRP    42      49.455  73.339   8.688  1.00 20.93       B_13
ATOM   1890  N   SER    43      51.432  72.987   9.710  1.00 20.63       B_13
ATOM   1892  CA  SER    43      51.007  73.601  10.968  1.00 22.47       B_13
ATOM   1893  CB  SER    43      51.955  73.231  12.116  1.00 10.00       B_13
ATOM   1894  OG  SER    43      53.265  73.716  11.891  1.00 33.50       B_13
ATOM   1896  C   SER    43      50.913  75.122  10.829  1.00 14.99       B_13
ATOM   1897  O   SER    43      50.224  75.784  11.595  1.00 11.58       B_13
ATOM   1898  N   ASP    44      51.613  75.667   9.843  1.00 26.20       B_13
ATOM   1900  CA  ASP    44      51.595  77.100   9.617  1.00 22.11       B_13
ATOM   1901  CB  ASP    44      52.620  77.485   8.549  1.00 11.09       B_13
ATOM   1902  CG  ASP    44      54.000  77.751   9.125  1.00 18.45       B_13
ATOM   1903  OD1 ASP    44      54.903  78.114   8.347  1.00 17.67       B_13
ATOM   1904  OD2 ASP    44      54.195  77.602  10.345  1.00 21.44       B_13
ATOM   1905  C   ASP    44      50.216  77.575   9.190  1.00 32.83       B_13
ATOM   1906  O   ASP    44      49.795  78.677   9.549  1.00 34.78       B_13
ATOM   1907  N   VAL    45      49.508  76.735   8.439  1.00 31.40       B_13
ATOM   1909  CA  VAL    45      48.191  77.094   7.932  1.00 14.00       B_13
ATOM   1910  CB  VAL    45      48.121  76.872   6.401  1.00 15.73       B_13
ATOM   1911  CG1 VAL    45      49.123  77.755   5.707  1.00 19.37       B_13
ATOM   1912  CG2 VAL    45      48.407  75.409   6.055  1.00 10.00       B_13
```

ATOM	1913	C	VAL	45	47.054	76.333	8.575	1.00	18.43	B_13
ATOM	1914	O	VAL	45	45.954	76.304	8.026	1.00	26.09	B_13
ATOM	1915	N	THR	46	47.295	75.754	9.747	1.00	18.49	B_13
ATOM	1917	CA	THR	46	46.262	74.963	10.408	1.00	21.92	B_13
ATOM	1918	CB	THR	46	46.222	73.529	9.751	1.00	27.61	B_13
ATOM	1919	OG1	THR	46	44.876	73.047	9.661	1.00	28.78	B_13
ATOM	1921	CG2	THR	46	47.054	72.550	10.522	1.00	10.65	B_13
ATOM	1922	C	THR	46	46.505	74.931	11.932	1.00	18.41	B_13
ATOM	1923	O	THR	46	47.554	75.363	12.411	1.00	18.63	B_13
ATOM	1924	N	PRO	47	45.519	74.467	12.717	1.00	16.81	B_13
ATOM	1925	CD	PRO	47	44.113	74.209	12.348	1.00	32.80	B_13
ATOM	1926	CA	PRO	47	45.691	74.407	14.169	1.00	13.66	B_13
ATOM	1927	CB	PRO	47	44.256	74.489	14.675	1.00	30.52	B_13
ATOM	1928	CG	PRO	47	43.519	73.692	13.638	1.00	29.25	B_13
ATOM	1929	C	PRO	47	46.346	73.105	14.622	1.00	28.40	B_13
ATOM	1930	O	PRO	47	46.037	72.597	15.705	1.00	29.19	B_13
ATOM	1931	N	LEU	48	47.220	72.547	13.784	1.00	27.10	B_13
ATOM	1933	CA	LEU	48	47.915	71.302	14.124	1.00	21.49	B_13
ATOM	1934	CB	LEU	48	48.087	70.418	12.885	1.00	16.21	B_13
ATOM	1935	CG	LEU	48	46.924	69.476	12.538	1.00	15.14	B_13
ATOM	1936	CD1	LEU	48	45.618	70.049	13.000	1.00	26.83	B_13
ATOM	1937	CD2	LEU	48	46.894	69.206	11.035	1.00	32.93	B_13
ATOM	1938	C	LEU	48	49.262	71.611	14.771	1.00	16.35	B_13
ATOM	1939	O	LEU	48	49.885	72.648	14.498	1.00	26.65	B_13
ATOM	1940	N	ASN	49	49.691	70.744	15.669	1.00	18.84	B_13
ATOM	1942	CA	ASN	49	50.956	70.940	16.354	1.00	25.67	B_13
ATOM	1943	CB	ASN	49	50.741	71.205	17.846	1.00	23.64	B_13
ATOM	1944	CG	ASN	49	49.734	72.301	18.100	1.00	23.64	B_13
ATOM	1945	OD1	ASN	49	48.895	72.192	18.989	1.00	33.47	B_13
ATOM	1946	ND2	ASN	49	49.796	73.359	17.305	1.00	37.40	B_13
ATOM	1949	C	ASN	49	51.695	69.643	16.195	1.00	22.08	B_13
ATOM	1950	O	ASN	49	51.087	68.577	16.252	1.00	23.48	B_13
ATOM	1951	N	PHE	50	52.994	69.723	15.951	1.00	25.59	B_13
ATOM	1953	CA	PHE	50	53.762	68.510	15.806	1.00	19.57	B_13
ATOM	1954	CB	PHE	50	54.258	68.343	14.380	1.00	12.47	B_13
ATOM	1955	CG	PHE	50	53.161	68.024	13.432	1.00	14.47	B_13
ATOM	1956	CD1	PHE	50	52.665	68.989	12.581	1.00	17.81	B_13
ATOM	1957	CD2	PHE	50	52.566	66.770	13.445	1.00	14.44	B_13
ATOM	1958	CE1	PHE	50	51.585	68.705	11.754	1.00	23.43	B_13
ATOM	1959	CE2	PHE	50	51.488	66.482	12.624	1.00	20.62	B_13
ATOM	1960	CZ	PHE	50	50.999	67.447	11.781	1.00	13.34	B_13
ATOM	1961	C	PHE	50	54.858	68.419	16.826	1.00	23.56	B_13
ATOM	1962	O	PHE	50	55.720	69.299	16.922	1.00	20.28	B_13
ATOM	1963	N	THR	51	54.728	67.387	17.651	1.00	26.45	B_13
ATOM	1965	CA	THR	51	55.650	67.090	18.725	1.00	29.37	B_13
ATOM	1966	CB	THR	51	54.851	66.834	20.024	1.00	28.17	B_13
ATOM	1967	OG1	THR	51	53.946	65.738	19.824	1.00	40.86	B_13
ATOM	1969	CG2	THR	51	54.032	68.078	20.393	1.00	25.37	B_13
ATOM	1970	C	THR	51	56.435	65.838	18.331	1.00	21.26	B_13
ATOM	1971	O	THR	51	55.849	64.849	17.882	1.00	17.45	B_13
ATOM	1972	N	ARG	52	57.755	65.889	18.477	1.00	15.17	B_13
ATOM	1974	CA	ARG	52	58.604	64.752	18.126	1.00	20.79	B_13
ATOM	1975	CB	ARG	52	59.868	65.241	17.429	1.00	20.81	B_13
ATOM	1976	CG	ARG	52	60.871	64.160	17.110	1.00	19.06	B_13
ATOM	1977	CD	ARG	52	62.208	64.808	16.880	1.00	22.17	B_13
ATOM	1978	NE	ARG	52	63.293	63.848	16.904	1.00	18.57	B_13
ATOM	1980	CZ	ARG	52	64.563	64.160	17.108	1.00	10.00	B_13
ATOM	1981	NH1	ARG	52	64.915	65.414	17.315	1.00	19.35	B_13
ATOM	1984	NH2	ARG	52	65.488	63.214	17.039	1.00	35.90	B_13
ATOM	1987	C	ARG	52	58.995	63.903	19.328	1.00	22.29	B_13
ATOM	1988	O	ARG	52	59.326	64.433	20.387	1.00	24.98	B_13
ATOM	1989	N	LEU	53	59.013	62.586	19.140	1.00	19.90	B_13
ATOM	1991	CA	LEU	53	59.378	61.660	20.203	1.00	27.02	B_13
ATOM	1992	CB	LEU	53	58.279	60.625	20.434	1.00	16.80	B_13
ATOM	1993	CG	LEU	53	56.859	61.138	20.639	1.00	23.45	B_13
ATOM	1994	CD1	LEU	53	55.943	59.943	20.884	1.00	24.07	B_13
ATOM	1995	CD2	LEU	53	56.801	62.143	21.785	1.00	21.02	B_13
ATOM	1996	C	LEU	53	60.657	60.944	19.615	1.00	15.06	B_13
ATOM	1997	O	LEU	53	60.822	60.539	18.671	1.00	13.89	B_13
ATOM	1998	N	HIS	54	61.532	60.750	20.792	1.00	19.96	B_13
ATOM	2000	CA	HIS	54	62.812	60.079	20.568	1.00	28.80	B_13
ATOM	2001	CB	HIS	54	63.848	60.604	21.569	1.00	19.40	B_13
ATOM	2002	CG	HIS	54	64.113	62.075	21.431	1.00	31.96	B_13
ATOM	2003	CD2	HIS	54	63.365	63.060	20.883	1.00	21.32	B_13
ATOM	2004	ND1	HIS	54	65.292	62.662	21.835	1.00	33.94	B_13
ATOM	2006	CE1	HIS	54	65.260	63.949	21.539	1.00	18.64	B_13
ATOM	2007	NE2	HIS	54	64.103	64.218	20.960	1.00	19.56	B_13

```
ATOM   2009  C   HIS   54      62.695  58.555  20.647  1.00 13.04      B_13
ATOM   2010  O   HIS   54      63.620  57.850  20.282  1.00 19.90      B_13
ATOM   2011  N   ASP   55      61.586  58.076  21.219  1.00 17.27      B_13
ATOM   2013  CA  ASP   55      61.303  56.648  21.366  1.00 25.79      B_13
ATOM   2014  CB  ASP   55      62.099  56.038  22.533  1.00 29.40      B_13
ATOM   2015  CG  ASP   55      63.443  55.428  22.076  1.00 29.64      B_13
ATOM   2016  OD1 ASP   55      63.517  54.906  20.942  1.00 33.28      B_13
ATOM   2017  OD2 ASP   55      64.437  55.469  22.831  1.00 31.99      B_13
ATOM   2018  C   ASP   55      59.807  56.460  21.567  1.00 24.99      B_13
ATOM   2019  O   ASP   55      59.079  57.445  21.677  1.00 21.06      B_13
ATOM   2020  N   GLY   56      59.358  55.207  21.559  1.00 22.90      B_13
ATOM   2022  CA  GLY   56      57.954  54.877  21.737  1.00 21.80      B_13
ATOM   2023  C   GLY   56      57.155  54.926  20.447  1.00 14.48      B_13
ATOM   2024  O   GLY   56      57.720  55.108  19.379  1.00 19.38      B_13
ATOM   2025  N   ILE   57      55.841  54.742  20.545  1.00 11.78      B_13
ATOM   2027  CA  ILE   57      54.944  54.809  19.389  1.00 16.25      B_13
ATOM   2028  CB  ILE   57      53.737  53.804  19.510  1.00 22.94      B_13
ATOM   2029  CG2 ILE   57      52.442  54.417  18.955  1.00 24.79      B_13
ATOM   2030  CG1 ILE   57      54.025  52.505  18.744  1.00 25.63      B_13
ATOM   2031  CD1 ILE   57      53.586  52.520  17.240  1.00 17.48      B_13
ATOM   2032  C   ILE   57      54.410  56.238  19.301  1.00 18.78      B_13
ATOM   2033  O   ILE   57      53.866  56.777  20.270  1.00 11.40      B_13
ATOM   2034  N   ALA   58      54.598  56.842  18.140  1.00 14.67      B_13
ATOM   2036  CA  ALA   58      54.139  58.200  17.857  1.00 17.04      B_13
ATOM   2037  CB  ALA   58      55.270  59.015  17.245  1.00 10.00      B_13
ATOM   2038  C   ALA   58      53.048  58.009  16.825  1.00 25.41      B_13
ATOM   2039  O   ALA   58      52.956  56.940  16.243  1.00 22.59      B_13
ATOM   2040  N   ASP   59      52.211  59.020  16.609  1.00 13.36      B_13
ATOM   2042  CA  ASP   59      51.156  58.927  15.606  1.00 24.67      B_13
ATOM   2043  CB  ASP   59      50.348  60.237  15.545  1.00 10.00      B_13
ATOM   2044  CG  ASP   59      49.743  60.631  16.899  1.00 12.93      B_13
ATOM   2045  OD1 ASP   59      49.922  61.788  17.327  1.00 32.89      B_13
ATOM   2046  OD2 ASP   59      49.076  59.793  17.541  1.00 21.52      B_13
ATOM   2047  C   ASP   59      51.784  58.653  14.242  1.00 11.46      B_13
ATOM   2048  O   ASP   59      51.378  57.736  13.531  1.00 16.58      B_13
ATOM   2049  N   ILE   60      52.791  59.445  13.899  1.00 24.90      B_13
ATOM   2051  CA  ILE   60      53.494  59.346  12.624  1.00 12.17      B_13
ATOM   2052  CB  ILE   60      53.620  60.738  11.975  1.00 10.91      B_13
ATOM   2053  CG2 ILE   60      54.289  60.641  10.588  1.00 10.70      B_13
ATOM   2054  CG1 ILE   60      52.228  61.367  11.851  1.00 18.58      B_13
ATOM   2055  CD1 ILE   60      52.219  62.870  11.726  1.00 12.00      B_13
ATOM   2056  C   ILE   60      54.881  58.750  12.841  1.00 12.93      B_13
ATOM   2057  O   ILE   60      55.788  59.392  13.365  1.00 16.39      B_13
ATOM   2058  N   MET   61      55.015  57.485  12.483  1.00 19.08      B_13
ATOM   2060  CA  MET   61      56.275  56.784  12.617  1.00 16.97      B_13
ATOM   2061  CB  MET   61      56.011  55.328  13.035  1.00 23.79      B_13
ATOM   2062  CG  MET   61      55.313  55.172  14.422  1.00 12.37      B_13
ATOM   2063  SD  MET   61      56.389  55.360  15.913  1.00 31.01      B_13
ATOM   2064  CE  MET   61      57.204  53.749  15.861  1.00 14.93      B_13
ATOM   2065  C   MET   61      56.995  56.888  11.265  1.00 12.72      B_13
ATOM   2066  O   MET   61      56.438  56.538  10.216  1.00 15.31      B_13
ATOM   2067  N   ILE   62      58.170  57.518  11.294  1.00 16.64      B_13
ATOM   2069  CA  ILE   62      58.978  57.739  10.097  1.00 27.48      B_13
ATOM   2070  CB  ILE   62      59.557  59.181  10.060  1.00 10.00      B_13
ATOM   2071  CG2 ILE   62      60.191  59.462   8.717  1.00 18.65      B_13
ATOM   2072  CG1 ILE   62      58.460  60.203  10.342  1.00 18.51      B_13
ATOM   2073  CD1 ILE   62      58.983  61.499  10.931  1.00 16.23      B_13
ATOM   2074  C   ILE   62      60.155  56.787  10.046  1.00 15.06      B_13
ATOM   2075  O   ILE   62      60.873  56.606  11.033  1.00 10.73      B_13
ATOM   2076  N   SER   63      60.398  56.230   8.873  1.00 19.40      B_13
ATOM   2078  CA  SER   63      61.513  55.321   8.722  1.00 13.31      B_13
ATOM   2079  CB  SER   63      61.111  53.888   9.123  1.00 17.28      B_13
ATOM   2080  OG  SER   63      59.985  53.435   8.391  1.00 13.66      B_13
ATOM   2082  C   SER   63      62.086  55.339   7.315  1.00 19.86      B_13
ATOM   2083  O   SER   63      61.441  55.766   6.347  1.00 20.93      B_13
ATOM   2084  N   PHE   64      63.338  54.914   7.237  1.00 17.78      B_13
ATOM   2086  CA  PHE   64      64.072  54.823   5.989  1.00 18.81      B_13
ATOM   2087  CB  PHE   64      65.409  55.553   6.105  1.00 16.50      B_13
ATOM   2088  CG  PHE   64      65.278  57.054   6.171  1.00 22.54      B_13
ATOM   2089  CD1 PHE   64      65.321  57.817   5.013  1.00 20.48      B_13
ATOM   2090  CD2 PHE   64      65.155  57.708   7.395  1.00 24.76      B_13
ATOM   2091  CE1 PHE   64      65.246  59.207   5.071  1.00 13.94      B_13
ATOM   2092  CE2 PHE   64      65.079  59.105   7.461  1.00 14.29      B_13
ATOM   2093  CZ  PHE   64      65.128  59.847   6.298  1.00 10.16      B_13
ATOM   2094  C   PHE   64      64.293  53.336   5.823  1.00 10.30      B_13
ATOM   2095  O   PHE   64      64.571  52.637   6.799  1.00 14.11      B_13
ATOM   2096  N   GLY   65      64.121  52.842   4.610  1.00 13.58      B_13
```

ATOM	2098	CA	GLY	65	64.306	51.426	4.392	1.00	14.88	B_13
ATOM	2099	C	GLY	65	64.400	51.117	2.922	1.00	14.95	B_13
ATOM	2100	O	GLY	65	64.047	51.947	2.088	1.00	12.61	B_13
ATOM	2101	N	ILE	66	64.860	49.922	2.587	1.00	10.00	B_13
ATOM	2103	CA	ILE	66	64.995	49.555	1.187	1.00	19.70	B_13
ATOM	2104	CB	ILE	66	66.483	49.344	0.791	1.00	18.92	B_13
ATOM	2105	CG2	ILE	66	67.301	50.628	1.073	1.00	10.00	B_13
ATOM	2106	CG1	ILE	66	67.078	48.178	1.582	1.00	14.64	B_13
ATOM	2107	CD1	ILE	66	68.381	47.662	1.004	1.00	17.53	B_13
ATOM	2108	C	ILE	66	64.195	48.296	0.900	1.00	15.98	B_13
ATOM	2109	O	ILE	66	63.877	47.543	1.806	1.00	20.10	B_13
ATOM	2110	N	LYS	67	63.773	48.148	-0.349	1.00	18.78	B_13
ATOM	2112	CA	LYS	67	63.019	46.980	-0.787	1.00	14.73	B_13
ATOM	2113	CB	LYS	67	63.986	45.827	-1.073	1.00	22.08	B_13
ATOM	2114	CG	LYS	67	65.107	46.142	-2.066	1.00	15.53	B_13
ATOM	2115	CD	LYS	67	64.591	46.325	-3.487	1.00	16.76	B_13
ATOM	2116	CE	LYS	67	65.573	45.763	-4.523	1.00	21.90	B_13
ATOM	2117	NZ	LYS	67	66.975	46.257	-4.394	1.00	28.03	B_13
ATOM	2121	C	LYS	67	61.945	46.548	0.218	1.00	16.24	B_13
ATOM	2122	O	LYS	67	61.136	47.360	0.649	1.00	10.25	B_13
ATOM	2123	N	GLU	68	61.968	45.293	0.630	1.00	10.00	B_13
ATOM	2125	CA	GLU	68	60.986	44.787	1.570	1.00	10.00	B_13
ATOM	2126	CB	GLU	68	61.004	43.257	1.505	1.00	31.44	B_13
ATOM	2127	CG	GLU	68	59.733	42.550	1.696	1.00	27.13	B_13
ATOM	2128	CD	GLU	68	58.723	42.720	0.524	1.00	12.88	B_13
ATOM	2129	OE1	GLU	68	59.106	42.180	-0.613	1.00	14.05	B_13
ATOM	2130	OE2	GLU	68	57.681	43.274	0.753	1.00	38.61	B_13
ATOM	2131	C	GLU	68	61.402	45.292	2.954	1.00	32.89	B_13
ATOM	2132	O	GLU	68	62.541	45.099	3.390	1.00	19.77	B_13
ATOM	2133	N	HIS	69	60.467	45.918	3.659	1.00	15.43	B_13
ATOM	2135	CA	HIS	69	60.777	46.473	4.964	1.00	10.00	B_13
ATOM	2136	CB	HIS	69	61.173	47.928	4.802	1.00	15.60	B_13
ATOM	2137	CG	HIS	69	60.151	48.731	4.063	1.00	18.06	B_13
ATOM	2138	CD2	HIS	69	59.131	49.509	4.498	1.00	25.01	B_13
ATOM	2139	ND1	HIS	69	60.055	48.709	2.689	1.00	21.79	B_13
ATOM	2141	CE1	HIS	69	59.023	49.430	2.308	1.00	19.43	B_13
ATOM	2142	NE2	HIS	69	58.438	49.932	3.384	1.00	19.23	B_13
ATOM	2143	C	HIS	69	59.655	46.396	5.978	1.00	16.27	B_13
ATOM	2144	O	HIS	69	59.689	47.099	6.969	1.00	13.47	B_13
ATOM	2145	N	GLY	70	58.610	45.629	5.719	1.00	21.21	B_13
ATOM	2147	CA	GLY	70	57.567	45.520	6.720	1.00	15.93	B_13
ATOM	2148	C	GLY	70	56.147	45.784	6.287	1.00	13.13	B_13
ATOM	2149	O	GLY	70	55.283	45.986	7.147	1.00	12.19	B_13
ATOM	2150	N	ASP	71	55.891	45.805	4.983	1.00	10.00	B_13
ATOM	2152	CA	ASP	71	54.540	46.030	4.480	1.00	17.84	B_13
ATOM	2153	CB	ASP	71	54.086	47.490	4.636	1.00	21.86	B_13
ATOM	2154	CG	ASP	71	54.946	48.480	3.881	1.00	13.38	B_13
ATOM	2155	OD1	ASP	71	54.896	49.644	4.291	1.00	10.00	B_13
ATOM	2156	OD2	ASP	71	55.633	48.135	2.897	1.00	10.00	B_13
ATOM	2157	C	ASP	71	54.313	45.557	3.064	1.00	27.18	B_13
ATOM	2158	O	ASP	71	55.221	45.068	2.416	1.00	16.61	B_13
ATOM	2159	N	PHE	72	53.103	45.759	2.564	1.00	10.00	B_13
ATOM	2161	CA	PHE	72	52.788	45.317	1.213	1.00	19.60	B_13
ATOM	2162	CB	PHE	72	51.292	45.017	1.099	1.00	16.43	B_13
ATOM	2163	CG	PHE	72	50.849	43.779	1.851	1.00	27.69	B_13
ATOM	2164	CD1	PHE	72	51.399	42.532	1.561	1.00	22.33	B_13
ATOM	2165	CD2	PHE	72	49.848	43.855	2.823	1.00	27.58	B_13
ATOM	2166	CE1	PHE	72	50.955	41.383	2.225	1.00	22.03	B_13
ATOM	2167	CE2	PHE	72	49.403	42.709	3.486	1.00	21.82	B_13
ATOM	2168	CZ	PHE	72	49.957	41.473	3.184	1.00	10.00	B_13
ATOM	2169	C	PHE	72	53.225	46.313	0.130	1.00	18.56	B_13
ATOM	2170	O	PHE	72	52.840	46.190	-1.048	1.00	14.78	B_13
ATOM	2171	N	TYR	73	54.079	47.260	0.513	1.00	10.93	B_13
ATOM	2173	CA	TYR	73	54.558	48.295	-0.416	1.00	13.87	B_13
ATOM	2174	CB	TYR	73	53.943	49.649	-0.048	1.00	22.69	B_13
ATOM	2175	CG	TYR	73	52.439	49.581	0.007	1.00	16.43	B_13
ATOM	2176	CD1	TYR	73	51.774	49.385	1.219	1.00	18.21	B_13
ATOM	2177	CE1	TYR	73	50.386	49.219	1.257	1.00	35.13	B_13
ATOM	2178	CD2	TYR	73	51.683	49.618	-1.165	1.00	15.77	B_13
ATOM	2179	CE2	TYR	73	50.300	49.456	-1.133	1.00	39.16	B_13
ATOM	2180	CZ	TYR	73	49.663	49.258	0.080	1.00	28.27	B_13
ATOM	2181	OH	TYR	73	48.301	49.122	0.106	1.00	33.06	B_13
ATOM	2183	C	TYR	73	56.088	48.349	-0.425	1.00	18.05	B_13
ATOM	2184	O	TYR	73	56.721	49.339	0.003	1.00	10.00	B_13
ATOM	2185	N	PRO	74	56.702	47.287	-0.953	1.00	13.76	B_13
ATOM	2186	CD	PRO	74	56.063	46.221	-1.740	1.00	14.21	B_13
ATOM	2187	CA	PRO	74	58.158	47.183	-1.024	1.00	21.66	B_13

ATOM	2188	CB	PRO	74	58.353	45.768	-1.569	1.00	15.88	B_13
ATOM	2189	CG	PRO	74	57.225	45.653	-2.540	1.00	13.95	B_13
ATOM	2190	C	PRO	74	58.747	48.226	-1.959	1.00	27.68	B_13
ATOM	2191	O	PRO	74	58.173	48.526	-3.012	1.00	21.90	B_13
ATOM	2192	N	PHE	75	59.883	48.794	-1.562	1.00	20.91	B_13
ATOM	2194	CA	PHE	75	60.554	49.773	-2.395	1.00	15.84	B_13
ATOM	2195	CB	PHE	75	61.498	50.637	-1.548	1.00	11.67	B_13
ATOM	2196	CG	PHE	75	60.765	51.589	-0.641	1.00	14.42	B_13
ATOM	2197	CD1	PHE	75	59.831	52.484	-1.162	1.00	16.56	B_13
ATOM	2198	CD2	PHE	75	60.976	51.574	0.726	1.00	10.00	B_13
ATOM	2199	CE1	PHE	75	59.119	53.345	-0.327	1.00	11.14	B_13
ATOM	2200	CE2	PHE	75	60.274	52.423	1.558	1.00	10.28	B_13
ATOM	2201	CZ	PHE	75	59.340	53.316	1.027	1.00	10.00	B_13
ATOM	2202	C	PHE	75	61.236	49.068	-3.573	1.00	14.23	B_13
ATOM	2203	O	PHE	75	61.357	47.837	-3.582	1.00	18.64	B_13
ATOM	2204	N	ASP	76	61.742	49.845	-4.526	1.00	12.83	B_13
ATOM	2206	CA	ASP	76	62.330	49.287	-5.740	1.00	20.69	B_13
ATOM	2207	CB	ASP	76	61.394	49.644	-6.911	1.00	14.28	B_13
ATOM	2208	CG	ASP	76	61.212	51.144	-7.080	1.00	14.37	B_13
ATOM	2209	OD1	ASP	76	61.361	51.882	-6.095	1.00	22.32	B_13
ATOM	2210	OD2	ASP	76	60.941	51.597	-8.202	1.00	15.92	B_13
ATOM	2211	C	ASP	76	63.764	49.698	-6.104	1.00	19.31	B_13
ATOM	2212	O	ASP	76	64.056	49.864	-7.278	1.00	18.67	B_13
ATOM	2213	N	GLY	77	64.653	49.902	-5.132	1.00	10.00	B_13
ATOM	2215	CA	GLY	77	65.997	50.326	-5.501	1.00	10.00	B_13
ATOM	2216	C	GLY	77	65.989	51.790	-5.970	1.00	16.22	B_13
ATOM	2217	O	GLY	77	64.967	52.487	-5.752	1.00	17.04	B_13
ATOM	2218	N	PRO	78	67.080	52.305	-6.589	1.00	12.53	B_13
ATOM	2219	CD	PRO	78	68.319	51.564	-6.856	1.00	12.24	B_13
ATOM	2220	CA	PRO	78	67.207	53.691	-7.086	1.00	11.81	B_13
ATOM	2221	CB	PRO	78	68.546	53.678	-7.816	1.00	10.00	B_13
ATOM	2222	CG	PRO	78	69.316	52.693	-7.066	1.00	12.78	B_13
ATOM	2223	C	PRO	78	66.093	54.146	-8.027	1.00	10.00	B_13
ATOM	2224	O	PRO	78	65.621	53.381	-8.853	1.00	27.46	B_13
ATOM	2225	N	SER	79	65.641	55.386	-7.852	1.00	19.14	B_13
ATOM	2227	CA	SER	79	64.568	55.963	-8.669	1.00	10.00	B_13
ATOM	2228	CB	SER	79	64.970	56.033	-10.148	1.00	20.11	B_13
ATOM	2229	OG	SER	79	63.982	56.723	-10.901	1.00	23.87	B_13
ATOM	2231	C	SER	79	63.231	55.215	-8.507	1.00	31.68	B_13
ATOM	2232	O	SER	79	63.074	54.356	-7.606	1.00	26.48	B_13
ATOM	2233	N	GLY	80	62.250	55.589	-9.327	1.00	10.00	B_13
ATOM	2235	CA	GLY	80	60.940	54.969	-9.260	1.00	10.07	B_13
ATOM	2236	C	GLY	80	60.293	55.412	-7.968	1.00	30.72	B_13
ATOM	2237	O	GLY	80	60.347	56.600	-7.643	1.00	20.65	B_13
ATOM	2238	N	LEU	81	59.779	54.452	-7.193	1.00	23.74	B_13
ATOM	2240	CA	LEU	81	59.135	54.752	-5.917	1.00	13.14	B_13
ATOM	2241	CB	LEU	81	58.661	53.481	-5.213	1.00	16.20	B_13
ATOM	2242	CG	LEU	81	57.393	52.775	-5.687	1.00	17.33	B_13
ATOM	2243	CD1	LEU	81	57.554	52.277	-7.096	1.00	28.67	B_13
ATOM	2244	CD2	LEU	81	57.103	51.617	-4.745	1.00	27.02	B_13
ATOM	2245	C	LEU	81	60.122	55.466	-5.019	1.00	14.51	B_13
ATOM	2246	O	LEU	81	61.264	55.016	-4.846	1.00	16.24	B_13
ATOM	2247	N	LEU	82	59.692	56.590	-4.470	1.00	11.33	B_13
ATOM	2249	CA	LEU	82	60.540	57.381	-3.594	1.00	17.52	B_13
ATOM	2250	CB	LEU	82	60.442	58.861	-3.986	1.00	18.51	B_13
ATOM	2251	CG	LEU	82	61.355	59.499	-5.044	1.00	15.37	B_13
ATOM	2252	CD1	LEU	82	61.800	58.504	-6.104	1.00	17.05	B_13
ATOM	2253	CD2	LEU	82	60.639	60.744	-5.659	1.00	16.87	B_13
ATOM	2254	C	LEU	82	60.172	57.203	-2.127	1.00	10.00	B_13
ATOM	2255	O	LEU	82	61.045	57.056	-1.275	1.00	19.90	B_13
ATOM	2256	N	ALA	83	58.876	57.201	-1.840	1.00	18.16	B_13
ATOM	2258	CA	ALA	83	58.378	57.077	-0.472	1.00	13.17	B_13
ATOM	2259	CB	ALA	83	58.762	58.322	0.327	1.00	10.00	B_13
ATOM	2260	C	ALA	83	56.846	56.925	-0.500	1.00	10.00	B_13
ATOM	2261	O	ALA	83	56.209	57.155	-1.541	1.00	10.73	B_13
ATOM	2262	N	HIS	84	56.268	56.619	0.662	1.00	10.00	B_13
ATOM	2264	CA	HIS	84	54.811	56.472	0.810	1.00	23.81	B_13
ATOM	2265	CB	HIS	84	54.270	55.188	0.157	1.00	30.45	B_13
ATOM	2266	CG	HIS	84	54.848	53.925	0.711	1.00	17.68	B_13
ATOM	2267	CD2	HIS	84	54.856	53.415	1.964	1.00	10.00	B_13
ATOM	2268	ND1	HIS	84	55.525	53.025	-0.076	1.00	14.94	B_13
ATOM	2270	CE1	HIS	84	55.933	52.015	0.666	1.00	29.72	B_13
ATOM	2271	NE2	HIS	84	55.543	52.224	1.912	1.00	13.81	B_13
ATOM	2272	C	HIS	84	54.363	56.547	2.258	1.00	12.82	B_13
ATOM	2273	O	HIS	84	55.099	56.148	3.166	1.00	20.02	B_13
ATOM	2274	N	ALA	85	53.161	57.076	2.464	1.00	28.38	B_13
ATOM	2276	CA	ALA	85	52.584	57.230	3.796	1.00	18.64	B_13

```
ATOM   2277  CB  ALA    85      52.638  58.705   4.223  1.00 13.89      B_13
ATOM   2278  C   ALA    85      51.138  56.716   3.837  1.00 10.00      B_13
ATOM   2279  O   ALA    85      50.434  56.728   2.828  1.00 10.00      B_13
ATOM   2280  N   PHE    86      50.676  56.322   5.016  1.00 14.76      B_13
ATOM   2282  CA  PHE    86      49.316  55.811   5.143  1.00 17.96      B_13
ATOM   2283  CB  PHE    86      49.286  54.592   6.084  1.00 15.86      B_13
ATOM   2284  CG  PHE    86      50.320  53.542   5.748  1.00 26.30      B_13
ATOM   2285  CD1 PHE    86      49.973  52.398   5.042  1.00 22.30      B_13
ATOM   2286  CD2 PHE    86      51.654  53.730   6.090  1.00 27.63      B_13
ATOM   2287  CE1 PHE    86      50.938  51.472   4.681  1.00 27.85      B_13
ATOM   2288  CE2 PHE    86      52.620  52.810   5.731  1.00 13.97      B_13
ATOM   2289  CZ  PHE    86      52.266  51.683   5.027  1.00 23.08      B_13
ATOM   2290  C   PHE    86      48.427  56.924   5.669  1.00 13.02      B_13
ATOM   2291  O   PHE    86      48.870  57.747   6.466  1.00 15.02      B_13
ATOM   2292  N   PRO    87      47.174  57.006   5.186  1.00 17.55      B_13
ATOM   2293  CD  PRO    87      46.565  56.165   4.146  1.00 10.17      B_13
ATOM   2294  CA  PRO    87      46.228  58.041   5.628  1.00 32.09      B_13
ATOM   2295  CB  PRO    87      44.961  57.720   4.819  1.00 18.55      B_13
ATOM   2296  CG  PRO    87      45.115  56.277   4.481  1.00 18.86      B_13
ATOM   2297  C   PRO    87      45.995  57.955   7.139  1.00 25.18      B_13
ATOM   2298  O   PRO    87      46.284  56.919   7.752  1.00 18.18      B_13
ATOM   2299  N   PRO    88      45.462  59.032   7.760  1.00 11.49      B_13
ATOM   2300  CD  PRO    88      45.015  60.303   7.164  1.00 10.00      B_13
ATOM   2301  CA  PRO    88      45.217  59.034   9.202  1.00 19.03      B_13
ATOM   2302  CB  PRO    88      44.399  60.302   9.402  1.00 14.16      B_13
ATOM   2303  CG  PRO    88      44.939  61.196   8.357  1.00 16.39      B_13
ATOM   2304  C   PRO    88      44.500  57.787   9.733  1.00 25.43      B_13
ATOM   2305  O   PRO    88      43.670  57.165   9.044  1.00 15.90      B_13
ATOM   2306  N   GLY    89      44.865  57.422  10.955  1.00 26.28      B_13
ATOM   2308  CA  GLY    89      44.299  56.264  11.606  1.00 25.32      B_13
ATOM   2309  C   GLY    89      45.343  55.713  12.546  1.00 34.38      B_13
ATOM   2310  O   GLY    89      46.485  56.164  12.498  1.00 23.28      B_13
ATOM   2311  N   PRO    90      44.977  54.774  13.437  1.00 13.87      B_13
ATOM   2312  CD  PRO    90      43.613  54.259  13.631  1.00 16.36      B_13
ATOM   2313  CA  PRO    90      45.898  54.164  14.398  1.00 10.34      B_13
ATOM   2314  CB  PRO    90      44.963  53.360  15.300  1.00 15.93      B_13
ATOM   2315  CG  PRO    90      43.870  52.975  14.373  1.00 23.25      B_13
ATOM   2316  C   PRO    90      46.942  53.299  13.711  1.00 18.38      B_13
ATOM   2317  O   PRO    90      46.875  53.064  12.505  1.00 26.81      B_13
ATOM   2318  N   ASN    91      47.903  52.831  14.502  1.00 26.63      B_13
ATOM   2320  CA  ASN    91      49.022  52.010  14.033  1.00 21.91      B_13
ATOM   2321  CB  ASN    91      48.740  50.500  14.081  1.00 18.89      B_13
ATOM   2322  CG  ASN    91      47.437  50.117  13.448  1.00 22.49      B_13
ATOM   2323  OD1 ASN    91      47.335  50.017  12.237  1.00 29.37      B_13
ATOM   2324  ND2 ASN    91      46.438  49.858  14.273  1.00 28.01      B_13
ATOM   2327  C   ASN    91      49.656  52.438  12.721  1.00 20.07      B_13
ATOM   2328  O   ASN    91      50.301  53.479  12.681  1.00 21.24      B_13
ATOM   2329  N   TYR    92      49.423  51.716  11.633  1.00 20.15      B_13
ATOM   2331  CA  TYR    92      50.052  52.081  10.367  1.00 18.70      B_13
ATOM   2332  CB  TYR    92      49.905  50.953   9.344  1.00 14.48      B_13
ATOM   2333  CG  TYR    92      50.906  49.821   9.567  1.00 24.41      B_13
ATOM   2334  CD1 TYR    92      52.266  50.003   9.287  1.00 27.39      B_13
ATOM   2335  CE1 TYR    92      53.198  48.979   9.471  1.00 18.14      B_13
ATOM   2336  CD2 TYR    92      50.499  48.571  10.044  1.00 28.07      B_13
ATOM   2337  CE2 TYR    92      51.427  47.529  10.230  1.00 36.50      B_13
ATOM   2338  CZ  TYR    92      52.778  47.741   9.940  1.00 43.64      B_13
ATOM   2339  OH  TYR    92      53.694  46.710  10.105  1.00 32.21      B_13
ATOM   2341  C   TYR    92      49.633  53.431   9.797  1.00 21.78      B_13
ATOM   2342  O   TYR    92      50.384  54.049   9.040  1.00 12.55      B_13
ATOM   2343  N   GLY    93      48.464  53.916  10.198  1.00 15.83      B_13
ATOM   2345  CA  GLY    93      48.015  55.216   9.732  1.00 11.69      B_13
ATOM   2346  C   GLY    93      48.971  56.326  10.134  1.00 18.60      B_13
ATOM   2347  O   GLY    93      49.561  56.300  11.227  1.00 22.00      B_13
ATOM   2348  N   GLY    94      49.205  57.258   9.216  1.00 10.27      B_13
ATOM   2350  CA  GLY    94      50.099  58.365   9.492  1.00 18.36      B_13
ATOM   2351  C   GLY    94      51.567  58.061   9.234  1.00 15.54      B_13
ATOM   2352  O   GLY    94      52.334  58.967   8.938  1.00 17.55      B_13
ATOM   2353  N   ASP    95      51.977  56.801   9.351  1.00 17.69      B_13
ATOM   2355  CA  ASP    95      53.386  56.457   9.134  1.00 19.67      B_13
ATOM   2356  CB  ASP    95      53.637  54.986   9.444  1.00 15.96      B_13
ATOM   2357  CG  ASP    95      53.346  54.634  10.900  1.00 25.37      B_13
ATOM   2358  OD1 ASP    95      53.627  53.484  11.297  1.00 16.05      B_13
ATOM   2359  OD2 ASP    95      52.835  55.488  11.656  1.00 14.66      B_13
ATOM   2360  C   ASP    95      53.896  56.808   7.733  1.00 17.15      B_13
ATOM   2361  O   ASP    95      53.162  56.711   6.746  1.00 19.09      B_13
ATOM   2362  N   ALA    96      55.166  57.198   7.662  1.00 18.71      B_13
ATOM   2364  CA  ALA    96      55.803  57.581   6.400  1.00 19.97      B_13
```

```
ATOM   2365  CB  ALA    96      56.098  59.095   6.379  1.00 22.61      B_13
ATOM   2366  C   ALA    96      57.088  56.784   6.204  1.00 25.63      B_13
ATOM   2367  O   ALA    96      57.948  56.724   7.095  1.00 12.54      B_13
ATOM   2368  N   HIS    97      57.211  56.166   5.035  1.00 13.27      B_13
ATOM   2370  CA  HIS    97      58.375  55.357   4.730  1.00 25.28      B_13
ATOM   2371  CB  HIS    97      57.955  53.905   4.464  1.00 10.00      B_13
ATOM   2372  CG  HIS    97      57.264  53.257   5.624  1.00 12.02      B_13
ATOM   2373  CD2 HIS    97      57.214  53.603   6.929  1.00 10.00      B_13
ATOM   2374  ND1 HIS    97      56.516  52.104   5.499  1.00 12.91      B_13
ATOM   2375  CE1 HIS    97      56.038  51.770   6.688  1.00 10.00      B_13
ATOM   2376  NE2 HIS    97      56.445  52.664   7.571  1.00 10.64      B_13
ATOM   2378  C   HIS    97      59.069  55.959   3.520  1.00 13.82      B_13
ATOM   2379  O   HIS    97      58.415  56.273   2.517  1.00 12.27      B_13
ATOM   2380  N   PHE    98      60.379  56.154   3.647  1.00 10.67      B_13
ATOM   2382  CA  PHE    98      61.224  56.718   2.595  1.00 15.67      B_13
ATOM   2383  CB  PHE    98      61.970  57.938   3.156  1.00 10.76      B_13
ATOM   2384  CG  PHE    98      61.055  59.025   3.627  1.00 17.93      B_13
ATOM   2385  CD1 PHE    98      60.730  60.082   2.786  1.00 18.92      B_13
ATOM   2386  CD2 PHE    98      60.476  58.974   4.893  1.00 14.14      B_13
ATOM   2387  CE1 PHE    98      59.833  61.066   3.201  1.00 22.42      B_13
ATOM   2388  CE2 PHE    98      59.574  59.962   5.315  1.00 10.00      B_13
ATOM   2389  CZ  PHE    98      59.257  61.002   4.469  1.00 10.00      B_13
ATOM   2390  C   PHE    98      62.218  55.669   2.064  1.00 26.64      B_13
ATOM   2391  O   PHE    98      62.882  54.969   2.851  1.00 13.27      B_13
ATOM   2392  N   ASP    99      62.331  55.577   0.738  1.00 12.24      B_13
ATOM   2394  CA  ASP    99      63.229  54.612   0.102  1.00 10.00      B_13
ATOM   2395  CB  ASP    99      62.884  54.471  -1.385  1.00 10.00      B_13
ATOM   2396  CG  ASP    99      63.615  53.311  -2.067  1.00 22.86      B_13
ATOM   2397  OD1 ASP    99      63.170  52.890  -3.160  1.00 11.60      B_13
ATOM   2398  OD2 ASP    99      64.624  52.806  -1.528  1.00 21.20      B_13
ATOM   2399  C   ASP    99      64.677  55.046   0.264  1.00 12.66      B_13
ATOM   2400  O   ASP    99      65.121  56.010  -0.366  1.00 18.37      B_13
ATOM   2401  N   ASP   100      65.439  54.289   1.046  1.00 12.86      B_13
ATOM   2403  CA  ASP   100      66.833  54.642   1.260  1.00 14.46      B_13
ATOM   2404  CB  ASP   100      67.308  54.271   2.660  1.00 17.70      B_13
ATOM   2405  CG  ASP   100      68.006  55.437   3.358  1.00 16.15      B_13
ATOM   2406  OD1 ASP   100      68.091  55.447   4.602  1.00 15.74      B_13
ATOM   2407  OD2 ASP   100      68.470  56.354   2.655  1.00 27.08      B_13
ATOM   2408  C   ASP   100      67.793  54.171   0.179  1.00 13.66      B_13
ATOM   2409  O   ASP   100      68.961  53.932   0.416  1.00 19.54      B_13
ATOM   2410  N   ASP   101      67.254  53.954  -1.010  1.00 12.83      B_13
ATOM   2412  CA  ASP   101      68.074  53.590  -2.164  1.00 10.00      B_13
ATOM   2413  CB  ASP   101      67.471  52.413  -2.933  1.00 10.00      B_13
ATOM   2414  CG  ASP   101      67.997  51.065  -2.449  1.00 16.87      B_13
ATOM   2415  OD1 ASP   101      67.232  50.089  -2.458  1.00 19.89      B_13
ATOM   2416  OD2 ASP   101      69.184  50.968  -2.066  1.00 18.51      B_13
ATOM   2417  C   ASP   101      68.108  54.858  -3.029  1.00 26.72      B_13
ATOM   2418  O   ASP   101      68.602  54.853  -4.172  1.00 12.11      B_13
ATOM   2419  N   GLU   102      67.500  55.922  -2.496  1.00 13.76      B_13
ATOM   2421  CA  GLU   102      67.462  57.217  -3.161  1.00 12.54      B_13
ATOM   2422  CB  GLU   102      66.135  57.958  -2.916  1.00 13.01      B_13
ATOM   2423  CG  GLU   102      64.873  57.257  -3.381  1.00 15.50      B_13
ATOM   2424  CD  GLU   102      64.973  56.707  -4.791  1.00 29.02      B_13
ATOM   2425  OE1 GLU   102      65.640  57.307  -5.665  1.00 12.78      B_13
ATOM   2426  OE2 GLU   102      64.399  55.635  -5.021  1.00 12.36      B_13
ATOM   2427  C   GLU   102      68.544  58.040  -2.505  1.00 14.96      B_13
ATOM   2428  O   GLU   102      68.939  57.760  -1.371  1.00 10.00      B_13
ATOM   2429  N   THR   103      69.030  59.039  -3.228  1.00 19.38      B_13
ATOM   2431  CA  THR   103      70.021  59.957  -2.693  1.00 16.49      B_13
ATOM   2432  CB  THR   103      70.973  60.490  -3.801  1.00 19.31      B_13
ATOM   2433  OG1 THR   103      71.661  59.384  -4.399  1.00 25.44      B_13
ATOM   2435  CG2 THR   103      72.006  61.462  -3.212  1.00 10.75      B_13
ATOM   2436  C   THR   103      69.180  61.104  -2.141  1.00 12.91      B_13
ATOM   2437  O   THR   103      68.414  61.727  -2.867  1.00 13.59      B_13
ATOM   2438  N   TRP   104      69.252  61.322  -0.842  1.00 20.60      B_13
ATOM   2440  CA  TRP   104      68.497  62.388  -0.237  1.00 13.62      B_13
ATOM   2441  CB  TRP   104      67.852  61.902   1.063  1.00 22.66      B_13
ATOM   2442  CG  TRP   104      66.837  60.808   0.870  1.00 22.99      B_13
ATOM   2443  CD2 TRP   104      65.505  60.953   0.347  1.00 27.35      B_13
ATOM   2444  CE2 TRP   104      64.936  59.654   0.287  1.00 12.61      B_13
ATOM   2445  CE3 TRP   104      64.741  62.054  -0.079  1.00 11.89      B_13
ATOM   2446  CD1 TRP   104      67.013  59.473   1.108  1.00 17.89      B_13
ATOM   2447  NE1 TRP   104      65.876  58.775   0.755  1.00 14.24      B_13
ATOM   2449  CZ2 TRP   104      63.632  59.429  -0.186  1.00 10.00      B_13
ATOM   2450  CZ3 TRP   104      63.445  61.832  -0.549  1.00 22.21      B_13
ATOM   2451  CH2 TRP   104      62.904  60.527  -0.598  1.00 23.31      B_13
ATOM   2452  C   TRP   104      69.416  63.570   0.033  1.00 16.43      B_13
```

ATOM	2453	O	TRP	104	70.520	63.380	0.526	1.00	11.13	B_13
ATOM	2454	N	THR	105	68.960	64.775	-0.322	1.00	19.48	B_13
ATOM	2456	CA	THR	105	69.716	66.015	-0.097	1.00	10.40	B_13
ATOM	2457	CB	THR	105	70.153	66.749	-1.398	1.00	10.00	B_13
ATOM	2458	OG1	THR	105	69.305	66.401	-2.501	1.00	18.53	B_13
ATOM	2460	CG2	THR	105	71.596	66.484	-1.709	1.00	34.62	B_13
ATOM	2461	C	THR	105	68.904	67.062	0.641	1.00	20.82	B_13
ATOM	2462	O	THR	105	67.686	66.952	0.768	1.00	15.93	B_13
ATOM	2463	N	SER	106	69.621	68.073	1.125	1.00	38.37	B_13
ATOM	2465	CA	SER	106	69.029	69.222	1.791	1.00	20.77	B_13
ATOM	2466	CB	SER	106	69.979	69.778	2.862	1.00	17.95	B_13
ATOM	2467	OG	SER	106	70.281	68.825	3.864	1.00	29.88	B_13
ATOM	2469	C	SER	106	68.889	70.245	0.657	1.00	19.23	B_13
ATOM	2470	O	SER	106	68.202	71.260	0.782	1.00	21.34	B_13
ATOM	2471	N	SER	107	69.577	69.981	-0.450	1.00	18.73	B_13
ATOM	2473	CA	SER	107	69.533	70.884	-1.592	1.00	20.92	B_13
ATOM	2474	CB	SER	107	70.945	71.380	-1.927	1.00	19.84	B_13
ATOM	2475	OG	SER	107	71.556	71.957	-0.788	1.00	27.31	B_13
ATOM	2477	C	SER	107	68.848	70.284	-2.828	1.00	18.68	B_13
ATOM	2478	O	SER	107	67.660	69.953	-2.771	1.00	21.51	B_13
ATOM	2479	N	SER	108	69.623	70.038	-3.888	1.00	18.53	B_13
ATOM	2481	CA	SER	108	69.091	69.544	-5.152	1.00	16.21	B_13
ATOM	2482	CB	SER	108	69.285	70.632	-6.205	1.00	29.10	B_13
ATOM	2483	OG	SER	108	70.665	70.969	-6.271	1.00	21.47	B_13
ATOM	2485	C	SER	108	69.645	68.260	-5.745	1.00	17.68	B_13
ATOM	2486	O	SER	108	68.964	67.618	-6.541	1.00	19.67	B_13
ATOM	2487	N	LYS	109	70.895	67.919	-5.448	1.00	11.70	B_13
ATOM	2489	CA	LYS	109	71.468	66.721	-6.047	1.00	10.00	B_13
ATOM	2490	CB	LYS	109	72.994	66.748	-5.989	1.00	18.86	B_13
ATOM	2491	CG	LYS	109	73.657	65.833	-7.013	1.00	16.33	B_13
ATOM	2492	CD	LYS	109	75.143	65.726	-6.740	1.00	11.58	B_13
ATOM	2493	CE	LYS	109	75.787	64.655	-7.606	1.00	27.43	B_13
ATOM	2494	NZ	LYS	109	77.218	64.492	-7.251	1.00	35.03	B_13
ATOM	2498	C	LYS	109	70.916	65.428	-5.444	1.00	29.39	B_13
ATOM	2499	O	LYS	109	71.432	64.905	-4.449	1.00	29.95	B_13
ATOM	2500	N	GLY	110	69.852	64.922	-6.055	1.00	14.77	B_13
ATOM	2502	CA	GLY	110	69.227	63.705	-5.576	1.00	24.08	B_13
ATOM	2503	C	GLY	110	67.793	64.105	-5.342	1.00	20.25	B_13
ATOM	2504	O	GLY	110	67.203	64.737	-6.198	1.00	16.21	B_13
ATOM	2505	N	TYR	111	67.248	63.772	-4.182	1.00	10.00	B_13
ATOM	2507	CA	TYR	111	65.879	64.130	-3.845	1.00	24.52	B_13
ATOM	2508	CB	TYR	111	65.030	62.868	-3.688	1.00	22.46	B_13
ATOM	2509	CG	TYR	111	64.676	62.244	-4.999	1.00	10.83	B_13
ATOM	2510	CD1	TYR	111	65.380	61.155	-5.483	1.00	25.38	B_13
ATOM	2511	CE1	TYR	111	65.068	60.592	-6.720	1.00	18.68	B_13
ATOM	2512	CD2	TYR	111	63.646	62.769	-5.776	1.00	16.02	B_13
ATOM	2513	CE2	TYR	111	63.328	62.223	-7.013	1.00	31.72	B_13
ATOM	2514	CZ	TYR	111	64.041	61.131	-7.473	1.00	23.68	B_13
ATOM	2515	OH	TYR	111	63.711	60.550	-8.666	1.00	20.96	B_13
ATOM	2517	C	TYR	111	65.856	64.944	-2.553	1.00	22.83	B_13
ATOM	2518	O	TYR	111	66.410	64.518	-1.538	1.00	11.66	B_13
ATOM	2519	N	ASN	112	65.278	66.140	-2.611	1.00	17.47	B_13
ATOM	2521	CA	ASN	112	65.180	67.006	-1.431	1.00	15.77	B_13
ATOM	2522	CB	ASN	112	64.658	68.401	-1.817	1.00	15.93	B_13
ATOM	2523	CG	ASN	112	64.694	69.384	-0.657	1.00	10.00	B_13
ATOM	2524	OD1	ASN	112	63.757	69.465	0.132	1.00	15.33	B_13
ATOM	2525	ND2	ASN	112	65.754	70.180	-0.586	1.00	13.70	B_13
ATOM	2528	C	ASN	112	64.214	66.329	-0.472	1.00	17.73	B_13
ATOM	2529	O	ASN	112	63.007	66.243	-0.737	1.00	12.61	B_13
ATOM	2530	N	LEU	113	64.755	65.830	0.630	1.00	16.28	B_13
ATOM	2532	CA	LEU	113	63.962	65.121	1.619	1.00	15.93	B_13
ATOM	2533	CB	LEU	113	64.841	64.703	2.804	1.00	11.93	B_13
ATOM	2534	CG	LEU	113	64.719	63.352	3.521	1.00	17.15	B_13
ATOM	2535	CD1	LEU	113	65.002	63.640	4.987	1.00	10.00	B_13
ATOM	2536	CD2	LEU	113	63.370	62.667	3.362	1.00	16.08	B_13
ATOM	2537	C	LEU	113	62.802	65.994	2.085	1.00	14.61	B_13
ATOM	2538	O	LEU	113	61.673	65.528	2.161	1.00	17.98	B_13
ATOM	2539	N	PHE	114	63.073	67.267	2.346	1.00	16.81	B_13
ATOM	2541	CA	PHE	114	62.056	68.212	2.791	1.00	15.65	B_13
ATOM	2542	CB	PHE	114	62.638	69.630	2.888	1.00	22.16	B_13
ATOM	2543	CG	PHE	114	61.596	70.714	2.882	1.00	12.27	B_13
ATOM	2544	CD1	PHE	114	60.804	70.952	4.004	1.00	19.93	B_13
ATOM	2545	CD2	PHE	114	61.378	71.470	1.746	1.00	13.56	B_13
ATOM	2546	CE1	PHE	114	59.813	71.932	3.984	1.00	17.08	B_13
ATOM	2547	CE2	PHE	114	60.398	72.441	1.726	1.00	13.79	B_13
ATOM	2548	CZ	PHE	114	59.615	72.666	2.848	1.00	10.70	B_13
ATOM	2549	C	PHE	114	60.860	68.220	1.842	1.00	19.55	B_13

```
ATOM   2550  O   PHE   114      59.714  68.156   2.285  1.00 15.97      B_13
ATOM   2551  N   LEU   115      61.135  68.309   0.543  1.00 13.35      B_13
ATOM   2553  CA  LEU   115      60.096  68.323  -0.485  1.00 17.91      B_13
ATOM   2554  CB  LEU   115      60.741  68.462  -1.868  1.00 24.65      B_13
ATOM   2555  CG  LEU   115      60.501  69.739  -2.679  1.00 22.70      B_13
ATOM   2556  CD1 LEU   115      61.033  70.939  -1.943  1.00 17.98      B_13
ATOM   2557  CD2 LEU   115      61.148  69.624  -4.048  1.00 28.50      B_13
ATOM   2558  C   LEU   115      59.235  67.042  -0.443  1.00 21.61      B_13
ATOM   2559  O   LEU   115      58.002  67.093  -0.344  1.00 13.99      B_13
ATOM   2560  N   VAL   116      59.898  65.895  -0.511  1.00 11.14      B_13
ATOM   2562  CA  VAL   116      59.199  64.616  -0.482  1.00 22.27      B_13
ATOM   2563  CB  VAL   116      60.163  63.421  -0.772  1.00 17.40      B_13
ATOM   2564  CG1 VAL   116      59.437  62.086  -0.629  1.00 23.09      B_13
ATOM   2565  CG2 VAL   116      60.741  63.534  -2.169  1.00 12.16      B_13
ATOM   2566  C   VAL   116      58.502  64.414   0.864  1.00 10.00      B_13
ATOM   2567  O   VAL   116      57.368  63.950   0.911  1.00 16.18      B_13
ATOM   2568  N   ALA   117      59.153  64.803   1.954  1.00 10.00      B_13
ATOM   2570  CA  ALA   117      58.585  64.640   3.297  1.00 19.50      B_13
ATOM   2571  CB  ALA   117      59.608  64.995   4.352  1.00 11.81      B_13
ATOM   2572  C   ALA   117      57.309  65.455   3.505  1.00 30.87      B_13
ATOM   2573  O   ALA   117      56.327  64.955   4.053  1.00 10.00      B_13
ATOM   2574  N   ALA   118      57.322  66.714   3.087  1.00 24.62      B_13
ATOM   2576  CA  ALA   118      56.140  67.553   3.222  1.00 20.76      B_13
ATOM   2577  CB  ALA   118      56.407  68.917   2.654  1.00 16.19      B_13
ATOM   2578  C   ALA   118      54.968  66.894   2.485  1.00 20.54      B_13
ATOM   2579  O   ALA   118      53.843  66.889   2.981  1.00 22.12      B_13
ATOM   2580  N   HIS   119      55.255  66.315   1.321  1.00 10.00      B_13
ATOM   2582  CA  HIS   119      54.259  65.647   0.489  1.00 17.27      B_13
ATOM   2583  CB  HIS   119      54.909  65.263  -0.860  1.00 11.16      B_13
ATOM   2584  CG  HIS   119      54.006  64.530  -1.813  1.00 26.59      B_13
ATOM   2585  CD2 HIS   119      53.377  63.335  -1.706  1.00 16.63      B_13
ATOM   2586  ND1 HIS   119      53.723  64.995  -3.085  1.00 12.44      B_13
ATOM   2588  CE1 HIS   119      52.961  64.124  -3.715  1.00 14.58      B_13
ATOM   2589  NE2 HIS   119      52.734  63.101  -2.901  1.00 26.44      B_13
ATOM   2590  C   HIS   119      53.722  64.419   1.227  1.00 17.00      B_13
ATOM   2591  O   HIS   119      52.510  64.218   1.331  1.00 17.01      B_13
ATOM   2592  N   GLU   120      54.626  63.607   1.751  1.00 10.31      B_13
ATOM   2594  CA  GLU   120      54.231  62.401   2.466  1.00 12.32      B_13
ATOM   2595  CB  GLU   120      55.463  61.627   2.961  1.00 15.34      B_13
ATOM   2596  CG  GLU   120      56.354  61.078   1.848  1.00 10.00      B_13
ATOM   2597  CD  GLU   120      55.574  60.260   0.867  1.00 18.64      B_13
ATOM   2598  OE1 GLU   120      55.598  60.565  -0.348  1.00 18.08      B_13
ATOM   2599  OE2 GLU   120      54.920  59.308   1.320  1.00 14.49      B_13
ATOM   2600  C   GLU   120      53.347  62.777   3.635  1.00 12.41      B_13
ATOM   2601  O   GLU   120      52.323  62.130   3.888  1.00 26.62      B_13
ATOM   2602  N   PHE   121      53.750  63.813   4.359  1.00 10.29      B_13
ATOM   2604  CA  PHE   121      52.993  64.286   5.506  1.00 14.37      B_13
ATOM   2605  CB  PHE   121      53.780  65.344   6.270  1.00 20.10      B_13
ATOM   2606  CG  PHE   121      55.057  64.827   6.852  1.00 24.55      B_13
ATOM   2607  CD1 PHE   121      56.037  65.700   7.292  1.00 10.00      B_13
ATOM   2608  CD2 PHE   121      55.292  63.454   6.936  1.00 23.62      B_13
ATOM   2609  CE1 PHE   121      57.247  65.212   7.813  1.00 18.59      B_13
ATOM   2610  CE2 PHE   121      56.488  62.954   7.448  1.00 15.21      B_13
ATOM   2611  CZ  PHE   121      57.472  63.834   7.888  1.00 25.40      B_13
ATOM   2612  C   PHE   121      51.607  64.791   5.110  1.00 16.63      B_13
ATOM   2613  O   PHE   121      50.676  64.760   5.921  1.00 26.80      B_13
ATOM   2614  N   GLY   122      51.471  65.238   3.864  1.00 11.98      B_13
ATOM   2616  CA  GLY   122      50.175  65.664   3.380  1.00 12.95      B_13
ATOM   2617  C   GLY   122      49.284  64.427   3.381  1.00 13.71      B_13
ATOM   2618  O   GLY   122      48.113  64.483   3.753  1.00 13.74      B_13
ATOM   2619  N   HIS   123      49.859  63.284   3.016  1.00 16.90      B_13
ATOM   2621  CA  HIS   123      49.126  62.009   3.008  1.00 24.90      B_13
ATOM   2622  CB  HIS   123      49.918  60.918   2.279  1.00 18.28      B_13
ATOM   2623  CG  HIS   123      49.945  61.084   0.794  1.00 21.62      B_13
ATOM   2624  CD2 HIS   123      50.889  60.764  -0.119  1.00 13.04      B_13
ATOM   2625  ND1 HIS   123      48.887  61.618   0.093  1.00 17.18      B_13
ATOM   2627  CE1 HIS   123      49.176  61.621  -1.195  1.00 16.02      B_13
ATOM   2628  NE2 HIS   123      50.386  61.108  -1.353  1.00 15.58      B_13
ATOM   2629  C   HIS   123      48.864  61.562   4.446  1.00 19.74      B_13
ATOM   2630  O   HIS   123      47.744  61.179   4.785  1.00 15.41      B_13
ATOM   2631  N   SER   124      49.904  61.627   5.284  1.00 13.32      B_13
ATOM   2633  CA  SER   124      49.813  61.270   6.695  1.00 27.50      B_13
ATOM   2634  CB  SER   124      51.131  61.582   7.425  1.00 18.63      B_13
ATOM   2635  OG  SER   124      52.221  60.837   6.925  1.00 13.32      B_13
ATOM   2637  C   SER   124      48.703  62.102   7.335  1.00 13.76      B_13
ATOM   2638  O   SER   124      48.061  61.677   8.306  1.00 20.65      B_13
ATOM   2639  N   LEU   125      48.481  63.300   6.814  1.00 13.33      B_13
```

ATOM	2641	CA	LEU	125	47.439	64.133	7.387	1.00	24.62	B_13
ATOM	2642	CB	LEU	125	47.893	65.592	7.436	1.00	20.76	B_13
ATOM	2643	CG	LEU	125	49.076	65.849	8.383	1.00	14.66	B_13
ATOM	2644	CD1	LEU	125	49.739	67.159	8.064	1.00	16.16	B_13
ATOM	2645	CD2	LEU	125	48.610	65.811	9.822	1.00	16.44	B_13
ATOM	2646	C	LEU	125	46.058	63.966	6.724	1.00	24.77	B_13
ATOM	2647	O	LEU	125	45.066	64.528	7.195	1.00	15.63	B_13
ATOM	2648	N	GLY	126	45.988	63.192	5.644	1.00	17.38	B_13
ATOM	2650	CA	GLY	126	44.700	62.968	5.001	1.00	22.41	B_13
ATOM	2651	C	GLY	126	44.453	63.487	3.603	1.00	13.20	B_13
ATOM	2652	O	GLY	126	43.349	63.366	3.096	1.00	20.86	B_13
ATOM	2653	N	LEU	127	45.452	64.079	2.972	1.00	12.39	B_13
ATOM	2655	CA	LEU	127	45.267	64.592	1.617	1.00	11.56	B_13
ATOM	2656	CB	LEU	127	45.965	65.947	1.467	1.00	19.19	B_13
ATOM	2657	CG	LEU	127	45.300	67.206	2.039	1.00	14.42	B_13
ATOM	2658	CD1	LEU	127	44.875	67.030	3.496	1.00	32.31	B_13
ATOM	2659	CD2	LEU	127	46.288	68.374	1.912	1.00	25.45	B_13
ATOM	2660	C	LEU	127	45.770	63.619	0.550	1.00	26.54	B_13
ATOM	2661	O	LEU	127	46.920	63.156	0.601	1.00	18.76	B_13
ATOM	2662	N	ASP	128	44.908	63.285	-0.407	1.00	28.54	B_13
ATOM	2664	CA	ASP	128	45.292	62.376	-1.480	1.00	10.89	B_13
ATOM	2665	CB	ASP	128	44.059	61.762	-2.136	1.00	15.95	B_13
ATOM	2666	CG	ASP	128	44.351	60.430	-2.794	1.00	23.44	B_13
ATOM	2667	OD1	ASP	128	43.377	59.735	-3.164	1.00	41.43	B_13
ATOM	2668	OD2	ASP	128	45.541	60.059	-2.918	1.00	18.12	B_13
ATOM	2669	C	ASP	128	46.060	63.203	-2.502	1.00	25.34	B_13
ATOM	2670	O	ASP	128	46.489	64.308	-2.213	1.00	16.36	B_13
ATOM	2671	N	HIS	129	46.283	62.645	-3.682	1.00	17.53	B_13
ATOM	2673	CA	HIS	129	47.001	63.366	-4.718	1.00	26.87	B_13
ATOM	2674	CB	HIS	129	47.495	62.398	-5.794	1.00	10.00	B_13
ATOM	2675	CG	HIS	129	48.729	61.645	-5.400	1.00	19.64	B_13
ATOM	2676	CD2	HIS	129	49.769	61.996	-4.609	1.00	19.96	B_13
ATOM	2677	ND1	HIS	129	49.012	60.373	-5.859	1.00	23.97	B_13
ATOM	2679	CE1	HIS	129	50.170	59.977	-5.372	1.00	17.95	B_13
ATOM	2680	NE2	HIS	129	50.658	60.944	-4.605	1.00	13.79	B_13
ATOM	2681	C	HIS	129	46.153	64.457	-5.360	1.00	39.97	B_13
ATOM	2682	O	HIS	129	45.011	64.220	-5.757	1.00	25.97	B_13
ATOM	2683	N	SER	130	46.743	65.640	-5.481	1.00	21.04	B_13
ATOM	2685	CA	SER	130	46.090	66.776	-6.109	1.00	16.72	B_13
ATOM	2686	CB	SER	130	46.847	68.058	-5.757	1.00	20.97	B_13
ATOM	2687	OG	SER	130	46.358	69.154	-6.502	1.00	25.52	B_13
ATOM	2689	C	SER	130	46.098	66.582	-7.622	1.00	24.66	B_13
ATOM	2690	O	SER	130	46.779	65.694	-8.145	1.00	29.24	B_13
ATOM	2691	N	LYS	131	45.315	67.403	-8.315	1.00	26.96	B_13
ATOM	2693	CA	LYS	131	45.253	67.358	-9.769	1.00	20.25	B_13
ATOM	2694	CB	LYS	131	43.796	67.379	-10.247	1.00	33.22	B_13
ATOM	2695	CG	LYS	131	43.159	68.775	-10.302	1.00	32.85	B_13
ATOM	2696	CD	LYS	131	43.335	69.436	-11.675	1.00	15.99	B_13
ATOM	2697	CE	LYS	131	43.023	70.919	-11.601	1.00	30.34	B_13
ATOM	2698	NZ	LYS	131	43.879	71.647	-10.600	1.00	30.44	B_13
ATOM	2702	C	LYS	131	45.998	68.602	-10.249	1.00	15.31	B_13
ATOM	2703	O	LYS	131	46.414	68.698	-11.402	1.00	30.72	B_13
ATOM	2704	N	ASP	132	46.191	69.536	-9.323	1.00	23.41	B_13
ATOM	2706	CA	ASP	132	46.869	70.798	-9.581	1.00	22.69	B_13
ATOM	2707	CB	ASP	132	46.641	71.726	-8.379	1.00	24.86	B_13
ATOM	2708	CG	ASP	132	46.819	73.200	-8.712	1.00	24.93	B_13
ATOM	2709	OD1	ASP	132	46.007	74.009	-8.208	1.00	29.71	B_13
ATOM	2710	OD2	ASP	132	47.766	73.555	-9.448	1.00	28.82	B_13
ATOM	2711	C	ASP	132	48.358	70.497	-9.728	1.00	14.97	B_13
ATOM	2712	O	ASP	132	49.047	70.235	-8.742	1.00	19.64	B_13
ATOM	2713	N	PRO	133	48.874	70.538	-10.964	1.00	16.94	B_13
ATOM	2714	CD	PRO	133	48.209	70.971	-12.199	1.00	21.42	B_13
ATOM	2715	CA	PRO	133	50.293	70.264	-11.215	1.00	19.34	B_13
ATOM	2716	CB	PRO	133	50.457	70.636	-12.690	1.00	20.48	B_13
ATOM	2717	CG	PRO	133	49.347	71.636	-12.929	1.00	21.80	B_13
ATOM	2718	C	PRO	133	51.237	71.059	-10.322	1.00	17.45	B_13
ATOM	2719	O	PRO	133	52.319	70.590	-10.006	1.00	23.30	B_13
ATOM	2720	N	GLY	134	50.799	72.246	-9.904	1.00	32.46	B_13
ATOM	2722	CA	GLY	134	51.610	73.104	-9.051	1.00	19.44	B_13
ATOM	2723	C	GLY	134	51.306	72.958	-7.569	1.00	22.33	B_13
ATOM	2724	O	GLY	134	51.556	73.877	-6.795	1.00	21.92	B_13
ATOM	2725	N	ALA	135	50.698	71.836	-7.190	1.00	34.71	B_13
ATOM	2727	CA	ALA	135	50.355	71.580	-5.794	1.00	18.35	B_13
ATOM	2728	CB	ALA	135	48.948	70.987	-5.690	1.00	14.30	B_13
ATOM	2729	C	ALA	135	51.370	70.616	-5.210	1.00	10.00	B_13
ATOM	2730	O	ALA	135	51.739	69.647	-5.858	1.00	17.52	B_13
ATOM	2731	N	LEU	136	51.727	70.842	-3.952	1.00	21.29	B_13

```
ATOM   2733  CA  LEU   136      52.692  70.015  -3.230  1.00 14.62      B_13
ATOM   2734  CB  LEU   136      52.738  70.458  -1.763  1.00 18.54      B_13
ATOM   2735  CG  LEU   136      54.007  70.308  -0.921  1.00 34.11      B_13
ATOM   2736  CD1 LEU   136      53.587  69.907   0.485  1.00 14.76      B_13
ATOM   2737  CD2 LEU   136      54.969  69.296  -1.508  1.00 11.64      B_13
ATOM   2738  C   LEU   136      52.232  68.564  -3.287  1.00 13.50      B_13
ATOM   2739  O   LEU   136      53.033  67.640  -3.238  1.00 19.04      B_13
ATOM   2740  N   MET   137      50.921  68.364  -3.281  1.00 17.54      B_13
ATOM   2742  CA  MET   137      50.360  67.019  -3.324  1.00 25.11      B_13
ATOM   2743  CB  MET   137      49.010  66.981  -2.599  1.00 19.80      B_13
ATOM   2744  CG  MET   137      49.083  67.312  -1.117  1.00 15.35      B_13
ATOM   2745  SD  MET   137      50.354  66.361  -0.262  1.00 11.22      B_13
ATOM   2746  CE  MET   137      49.882  64.680  -0.764  1.00 13.90      B_13
ATOM   2747  C   MET   137      50.254  66.387  -4.721  1.00 28.08      B_13
ATOM   2748  O   MET   137      49.730  65.268  -4.863  1.00 12.18      B_13
ATOM   2749  N   PHE   138      50.771  67.070  -5.743  1.00 10.00      B_13
ATOM   2751  CA  PHE   138      50.751  66.528  -7.097  1.00 12.27      B_13
ATOM   2752  CB  PHE   138      51.327  67.523  -8.094  1.00 19.38      B_13
ATOM   2753  CG  PHE   138      51.051  67.175  -9.534  1.00 25.74      B_13
ATOM   2754  CD1 PHE   138      52.090  67.077 -10.448  1.00 19.74      B_13
ATOM   2755  CD2 PHE   138      49.747  67.007  -9.990  1.00 24.46      B_13
ATOM   2756  CE1 PHE   138      51.843  66.824 -11.786  1.00 19.54      B_13
ATOM   2757  CE2 PHE   138      49.495  66.750 -11.335  1.00 24.12      B_13
ATOM   2758  CZ  PHE   138      50.544  66.664 -12.230  1.00 18.15      B_13
ATOM   2759  C   PHE   138      51.619  65.269  -7.068  1.00 25.93      B_13
ATOM   2760  O   PHE   138      52.658  65.226  -6.414  1.00 12.50      B_13
ATOM   2761  N   PRO   139      51.166  64.194  -7.714  1.00 25.17      B_13
ATOM   2762  CD  PRO   139      49.870  64.004  -8.392  1.00 10.00      B_13
ATOM   2763  CA  PRO   139      51.950  62.956  -7.713  1.00 18.48      B_13
ATOM   2764  CB  PRO   139      50.981  61.946  -8.339  1.00 15.96      B_13
ATOM   2765  CG  PRO   139      50.140  62.798  -9.250  1.00 18.82      B_13
ATOM   2766  C   PRO   139      53.299  62.950  -8.430  1.00 17.22      B_13
ATOM   2767  O   PRO   139      53.849  61.876  -8.661  1.00 36.93      B_13
ATOM   2768  N   ILE   140      53.844  64.114  -8.767  1.00 24.48      B_13
ATOM   2770  CA  ILE   140      55.118  64.155  -9.477  1.00 20.03      B_13
ATOM   2771  CB  ILE   140      54.996  64.807 -10.892  1.00 18.71      B_13
ATOM   2772  CG2 ILE   140      56.334  64.709 -11.639  1.00 23.96      B_13
ATOM   2773  CG1 ILE   140      53.932  64.113 -11.724  1.00 24.68      B_13
ATOM   2774  CD1 ILE   140      53.861  64.669 -13.125  1.00 25.83      B_13
ATOM   2775  C   ILE   140      56.109  64.992  -8.700  1.00 27.87      B_13
ATOM   2776  O   ILE   140      55.758  66.043  -8.248  1.00 22.39      B_13
ATOM   2777  N   TYR   141      57.332  64.512  -8.535  1.00 12.36      B_13
ATOM   2779  CA  TYR   141      58.350  65.281  -7.834  1.00 21.85      B_13
ATOM   2780  CB  TYR   141      59.418  64.353  -7.266  1.00 15.16      B_13
ATOM   2781  CG  TYR   141      60.592  65.096  -6.672  1.00 15.65      B_13
ATOM   2782  CD1 TYR   141      61.755  65.306  -7.407  1.00 18.56      B_13
ATOM   2783  CE1 TYR   141      62.836  65.967  -6.859  1.00 10.00      B_13
ATOM   2784  CD2 TYR   141      60.546  65.576  -5.366  1.00 11.42      B_13
ATOM   2785  CE2 TYR   141      61.626  66.236  -4.814  1.00 13.45      B_13
ATOM   2786  CZ  TYR   141      62.770  66.429  -5.567  1.00 10.00      B_13
ATOM   2787  OH  TYR   141      63.841  67.109  -5.016  1.00 18.97      B_13
ATOM   2789  C   TYR   141      59.042  66.270  -8.776  1.00 19.52      B_13
ATOM   2790  O   TYR   141      59.709  65.859  -9.727  1.00 21.37      B_13
ATOM   2791  N   THR   142      58.932  67.556  -8.465  1.00 23.99      B_13
ATOM   2793  CA  THR   142      59.573  68.616  -9.238  1.00 19.53      B_13
ATOM   2794  CB  THR   142      58.515  69.578  -9.807  1.00 10.00      B_13
ATOM   2795  OG1 THR   142      57.704  68.880 -10.756  1.00 37.02      B_13
ATOM   2797  CG2 THR   142      59.151  70.757 -10.457  1.00 34.35      B_13
ATOM   2798  C   THR   142      60.483  69.332  -8.235  1.00 19.89      B_13
ATOM   2799  O   THR   142      60.120  69.513  -7.076  1.00 25.67      B_13
ATOM   2800  N   TYR   143      61.699  69.677  -8.643  1.00 30.64      B_13
ATOM   2802  CA  TYR   143      62.609  70.344  -7.707  1.00 32.54      B_13
ATOM   2803  CB  TYR   143      64.091  70.190  -8.108  1.00 26.34      B_13
ATOM   2804  CG  TYR   143      65.008  71.048  -7.244  1.00 10.69      B_13
ATOM   2805  CD1 TYR   143      65.066  70.866  -5.852  1.00 16.37      B_13
ATOM   2806  CE1 TYR   143      65.801  71.738  -5.035  1.00 26.03      B_13
ATOM   2807  CD2 TYR   143      65.714  72.114  -7.795  1.00 17.36      B_13
ATOM   2808  CE2 TYR   143      66.451  73.006  -6.981  1.00 15.32      B_13
ATOM   2809  CZ  TYR   143      66.489  72.810  -5.610  1.00 10.00      B_13
ATOM   2810  OH  TYR   143      67.184  73.665  -4.790  1.00 27.84      B_13
ATOM   2812  C   TYR   143      62.330  71.815  -7.456  1.00 24.77      B_13
ATOM   2813  O   TYR   143      62.201  72.611  -8.399  1.00 26.19      B_13
ATOM   2814  N   THR   144      62.292  72.160  -6.170  1.00 22.23      B_13
ATOM   2816  CA  THR   144      62.103  73.533  -5.727  1.00 33.68      B_13
ATOM   2817  CB  THR   144      60.668  73.814  -5.189  1.00 28.06      B_13
ATOM   2818  OG1 THR   144      60.277  72.812  -4.241  1.00 38.14      B_13
ATOM   2820  CG2 THR   144      59.681  73.857  -6.346  1.00 48.73      B_13
```

ATOM	2821	C	THR	144	63.178	73.893	-4.695	1.00	35.52	B_13
ATOM	2822	O	THR	144	64.207	74.465	-5.064	1.00	39.57	B_13
ATOM	2823	N	GLY	145	62.967	73.552	-3.422	1.00	35.95	B_13
ATOM	2825	CA	GLY	145	63.967	73.872	-2.407	1.00	35.01	B_13
ATOM	2826	C	GLY	145	63.509	74.025	-0.965	1.00	26.81	B_13
ATOM	2827	O	GLY	145	62.566	74.773	-0.670	1.00	40.81	B_13
ATOM	2828	N	LYS	146	64.302	73.439	-0.066	1.00	27.13	B_13
ATOM	2830	CA	LYS	146	64.071	73.423	1.389	1.00	23.89	B_13
ATOM	2831	CB	LYS	146	65.163	72.548	2.049	1.00	29.08	B_13
ATOM	2832	CG	LYS	146	64.992	72.209	3.524	1.00	19.99	B_13
ATOM	2833	CD	LYS	146	66.079	71.224	3.913	1.00	20.44	B_13
ATOM	2834	CE	LYS	146	66.181	71.010	5.402	1.00	24.16	B_13
ATOM	2835	NZ	LYS	146	67.250	69.987	5.727	1.00	23.37	B_13
ATOM	2839	C	LYS	146	63.926	74.778	2.124	1.00	18.98	B_13
ATOM	2840	O	LYS	146	63.900	74.831	3.353	1.00	28.15	B_13
ATOM	2841	N	SER	147	63.826	75.871	1.382	1.00	35.50	B_13
ATOM	2843	CA	SER	147	63.661	77.185	1.992	1.00	31.59	B_13
ATOM	2844	CB	SER	147	64.988	77.673	2.594	1.00	27.05	B_13
ATOM	2845	OG	SER	147	65.996	77.756	1.586	1.00	48.28	B_13
ATOM	2847	C	SER	147	63.203	78.131	0.902	1.00	27.12	B_13
ATOM	2848	O	SER	147	62.743	79.251	1.168	1.00	33.75	B_13
ATOM	2849	N	HIS	148	63.248	77.644	-0.332	1.00	25.13	B_13
ATOM	2851	CA	HIS	148	62.872	78.465	-1.463	1.00	23.42	B_13
ATOM	2852	CB	HIS	148	63.704	78.076	-2.678	1.00	17.40	B_13
ATOM	2853	CG	HIS	148	65.174	78.020	-2.398	1.00	45.97	B_13
ATOM	2854	CD2	HIS	148	66.204	77.524	-3.121	1.00	27.24	B_13
ATOM	2855	ND1	HIS	148	65.724	78.476	-1.213	1.00	43.49	B_13
ATOM	2857	CE1	HIS	148	67.024	78.253	-1.218	1.00	30.28	B_13
ATOM	2858	NE2	HIS	148	67.342	77.676	-2.366	1.00	45.28	B_13
ATOM	2860	C	HIS	148	61.381	78.433	-1.796	1.00	47.15	B_13
ATOM	2861	O	HIS	148	60.936	79.166	-2.704	1.00	40.97	B_13
ATOM	2862	N	PHE	149	60.601	77.636	-1.053	1.00	48.76	B_13
ATOM	2864	CA	PHE	149	59.170	77.557	-1.347	1.00	32.44	B_13
ATOM	2865	CB	PHE	149	58.856	76.364	-2.269	1.00	27.77	B_13
ATOM	2866	CG	PHE	149	58.415	76.781	-3.657	1.00	24.63	B_13
ATOM	2867	CD1	PHE	149	57.826	75.874	-4.520	1.00	25.66	B_13
ATOM	2868	CD2	PHE	149	58.550	78.106	-4.072	1.00	30.89	B_13
ATOM	2869	CE1	PHE	149	57.376	76.277	-5.767	1.00	17.10	B_13
ATOM	2870	CE2	PHE	149	58.104	78.520	-5.311	1.00	18.57	B_13
ATOM	2871	CZ	PHE	149	57.513	77.608	-6.166	1.00	30.20	B_13
ATOM	2872	C	PHE	149	58.061	77.791	-0.308	1.00	27.40	B_13
ATOM	2873	O	PHE	149	58.299	77.971	0.892	1.00	29.69	B_13
ATOM	2874	N	MET	150	56.836	77.729	-0.822	1.00	28.66	B_13
ATOM	2876	CA	MET	150	55.621	78.027	-0.094	1.00	20.63	B_13
ATOM	2877	CB	MET	150	55.251	79.431	-0.503	1.00	25.60	B_13
ATOM	2878	CG	MET	150	55.599	79.691	-1.989	1.00	23.95	B_13
ATOM	2879	SD	MET	150	57.336	80.086	-2.296	1.00	76.68	B_13
ATOM	2880	CE	MET	150	57.209	81.473	-3.385	1.00	21.07	B_13
ATOM	2881	C	MET	150	54.436	77.118	-0.450	1.00	30.58	B_13
ATOM	2882	O	MET	150	54.104	76.948	-1.628	1.00	16.91	B_13
ATOM	2883	N	LEU	151	53.727	76.664	0.581	1.00	36.94	B_13
ATOM	2885	CA	LEU	151	52.576	75.772	0.431	1.00	25.68	B_13
ATOM	2886	CB	LEU	151	51.968	75.474	1.807	1.00	23.46	B_13
ATOM	2887	CG	LEU	151	51.087	74.232	1.927	1.00	24.21	B_13
ATOM	2888	CD1	LEU	151	51.936	72.998	1.657	1.00	21.54	B_13
ATOM	2889	CD2	LEU	151	50.487	74.150	3.314	1.00	19.89	B_13
ATOM	2890	C	LEU	151	51.498	76.322	-0.491	1.00	17.09	B_13
ATOM	2891	O	LEU	151	50.795	77.267	-0.136	1.00	35.38	B_13
ATOM	2892	N	PRO	152	51.338	75.727	-1.686	1.00	16.90	B_13
ATOM	2893	CD	PRO	152	52.154	74.643	-2.255	1.00	25.80	B_13
ATOM	2894	CA	PRO	152	50.334	76.170	-2.653	1.00	29.65	B_13
ATOM	2895	CB	PRO	152	50.447	75.110	-3.749	1.00	24.68	B_13
ATOM	2896	CG	PRO	152	51.892	74.791	-3.722	1.00	14.34	B_13
ATOM	2897	C	PRO	152	48.910	76.261	-2.087	1.00	10.00	B_13
ATOM	2898	O	PRO	152	48.543	75.505	-1.184	1.00	20.25	B_13
ATOM	2899	N	ASP	153	48.117	77.180	-2.639	1.00	19.53	B_13
ATOM	2901	CA	ASP	153	46.723	77.387	-2.226	1.00	15.90	B_13
ATOM	2902	CB	ASP	153	45.986	78.304	-3.213	1.00	22.34	B_13
ATOM	2903	CG	ASP	153	46.418	79.741	-3.115	1.00	28.86	B_13
ATOM	2904	OD1	ASP	153	47.016	80.115	-2.074	1.00	35.34	B_13
ATOM	2905	OD2	ASP	153	46.142	80.494	-4.084	1.00	30.09	B_13
ATOM	2906	C	ASP	153	45.953	76.084	-2.169	1.00	27.31	B_13
ATOM	2907	O	ASP	153	45.309	75.783	-1.167	1.00	23.50	B_13
ATOM	2908	N	ASP	154	46.000	75.339	-3.276	1.00	25.51	B_13
ATOM	2910	CA	ASP	154	45.316	74.063	-3.392	1.00	20.91	B_13
ATOM	2911	CB	ASP	154	45.745	73.364	-4.682	1.00	14.23	B_13
ATOM	2912	CG	ASP	154	45.033	72.062	-4.885	1.00	22.95	B_13

ATOM	2913	OD1	ASP	154	45.590	71.026	-4.516	1.00	17.80	B_13
ATOM	2914	OD2	ASP	154	43.904	72.076	-5.388	1.00	19.14	B_13
ATOM	2915	C	ASP	154	45.551	73.155	-2.173	1.00	26.95	B_13
ATOM	2916	O	ASP	154	44.629	72.491	-1.696	1.00	22.92	B_13
ATOM	2917	N	ASP	155	46.776	73.155	-1.654	1.00	23.56	B_13
ATOM	2919	CA	ASP	155	47.110	72.338	-0.490	1.00	28.69	B_13
ATOM	2920	CB	ASP	155	48.618	72.118	-0.388	1.00	12.87	B_13
ATOM	2921	CG	ASP	155	49.208	71.566	-1.676	1.00	24.35	B_13
ATOM	2922	OD1	ASP	155	49.705	72.369	-2.500	1.00	27.89	B_13
ATOM	2923	OD2	ASP	155	49.152	70.335	-1.875	1.00	16.96	B_13
ATOM	2924	C	ASP	155	46.582	72.976	0.781	1.00	25.41	B_13
ATOM	2925	O	ASP	155	46.055	72.275	1.656	1.00	13.36	B_13
ATOM	2926	N	VAL	156	46.733	74.296	0.891	1.00	16.99	B_13
ATOM	2928	CA	VAL	156	46.222	75.021	2.053	1.00	22.26	B_13
ATOM	2929	CB	VAL	156	46.340	76.571	1.901	1.00	25.69	B_13
ATOM	2930	CG1	VAL	156	45.811	77.249	3.158	1.00	14.95	B_13
ATOM	2931	CG2	VAL	156	47.768	77.007	1.641	1.00	17.52	B_13
ATOM	2932	C	VAL	156	44.727	74.705	2.129	1.00	10.00	B_13
ATOM	2933	O	VAL	156	44.224	74.234	3.145	1.00	22.47	B_13
ATOM	2934	N	GLN	157	44.033	74.980	1.029	1.00	16.19	B_13
ATOM	2936	CA	GLN	157	42.604	74.758	0.930	1.00	17.97	B_13
ATOM	2937	CB	GLN	157	42.108	75.039	-0.497	1.00	17.10	B_13
ATOM	2938	CG	GLN	157	40.804	75.852	-0.547	1.00	26.00	B_13
ATOM	2939	CD	GLN	157	40.949	77.284	-0.005	1.00	25.84	B_13
ATOM	2940	OE1	GLN	157	41.218	77.505	1.177	1.00	39.61	B_13
ATOM	2941	NE2	GLN	157	40.744	78.255	-0.875	1.00	32.22	B_13
ATOM	2944	C	GLN	157	42.347	73.324	1.309	1.00	18.69	B_13
ATOM	2945	O	GLN	157	41.368	73.015	1.982	1.00	10.00	B_13
ATOM	2946	N	GLY	158	43.272	72.460	0.903	1.00	31.05	B_13
ATOM	2948	CA	GLY	158	43.156	71.053	1.205	1.00	21.69	B_13
ATOM	2949	C	GLY	158	43.129	70.738	2.684	1.00	13.51	B_13
ATOM	2950	O	GLY	158	42.108	70.263	3.182	1.00	14.91	B_13
ATOM	2951	N	ILE	159	44.224	71.006	3.398	1.00	19.34	B_13
ATOM	2953	CA	ILE	159	44.268	70.686	4.827	1.00	19.14	B_13
ATOM	2954	CB	ILE	159	45.669	70.880	5.503	1.00	12.57	B_13
ATOM	2955	CG2	ILE	159	46.268	69.542	5.960	1.00	19.22	B_13
ATOM	2956	CG1	ILE	159	46.603	71.702	4.633	1.00	31.62	B_13
ATOM	2957	CD1	ILE	159	46.426	73.177	4.824	1.00	25.87	B_13
ATOM	2958	C	ILE	159	43.235	71.461	5.610	1.00	21.87	B_13
ATOM	2959	O	ILE	159	42.691	70.952	6.592	1.00	21.02	B_13
ATOM	2960	N	GLN	160	42.959	72.689	5.186	1.00	12.08	B_13
ATOM	2962	CA	GLN	160	41.967	73.483	5.874	1.00	11.43	B_13
ATOM	2963	CB	GLN	160	41.949	74.916	5.346	1.00	29.25	B_13
ATOM	2964	CG	GLN	160	43.158	75.737	5.827	1.00	22.01	B_13
ATOM	2965	CD	GLN	160	43.098	77.199	5.416	1.00	18.77	B_13
ATOM	2966	OE1	GLN	160	42.260	77.593	4.607	1.00	36.02	B_13
ATOM	2967	NE2	GLN	160	43.997	78.004	5.965	1.00	28.49	B_13
ATOM	2970	C	GLN	160	40.596	72.820	5.772	1.00	22.28	B_13
ATOM	2971	O	GLN	160	39.855	72.786	6.754	1.00	14.16	B_13
ATOM	2972	N	SER	161	40.304	72.183	4.634	1.00	32.89	B_13
ATOM	2974	CA	SER	161	39.005	71.537	4.474	1.00	29.25	B_13
ATOM	2975	CB	SER	161	38.847	70.901	3.085	1.00	19.70	B_13
ATOM	2976	OG	SER	161	39.594	69.706	2.946	1.00	24.88	B_13
ATOM	2978	C	SER	161	38.831	70.503	5.566	1.00	22.08	B_13
ATOM	2979	O	SER	161	37.745	70.340	6.118	1.00	26.26	B_13
ATOM	2980	N	LEU	162	39.931	69.852	5.919	1.00	19.14	B_13
ATOM	2982	CA	LEU	162	39.913	68.829	6.953	1.00	29.17	B_13
ATOM	2983	CB	LEU	162	41.081	67.852	6.767	1.00	12.08	B_13
ATOM	2984	CG	LEU	162	40.982	66.666	5.812	1.00	20.09	B_13
ATOM	2985	CD1	LEU	162	40.661	67.184	4.478	1.00	24.51	B_13
ATOM	2986	CD2	LEU	162	42.299	65.884	5.794	1.00	27.00	B_13
ATOM	2987	C	LEU	162	39.965	69.392	8.364	1.00	24.75	B_13
ATOM	2988	O	LEU	162	39.047	69.191	9.162	1.00	22.04	B_13
ATOM	2989	N	TYR	163	41.015	70.151	8.652	1.00	20.72	B_13
ATOM	2991	CA	TYR	163	41.211	70.689	9.980	1.00	10.00	B_13
ATOM	2992	CB	TYR	163	42.695	70.595	10.343	1.00	10.95	B_13
ATOM	2993	CG	TYR	163	43.221	69.167	10.209	1.00	10.00	B_13
ATOM	2994	CD1	TYR	163	43.114	68.261	11.264	1.00	37.53	B_13
ATOM	2995	CE1	TYR	163	43.452	66.913	11.103	1.00	26.00	B_13
ATOM	2996	CD2	TYR	163	43.703	68.689	8.990	1.00	23.78	B_13
ATOM	2997	CE2	TYR	163	44.048	67.342	8.822	1.00	17.88	B_13
ATOM	2998	CZ	TYR	163	43.914	66.461	9.879	1.00	24.28	B_13
ATOM	2999	OH	TYR	163	44.210	65.121	9.711	1.00	13.27	B_13
ATOM	3001	C	TYR	163	40.634	72.085	10.187	1.00	26.45	B_13
ATOM	3002	O	TYR	163	39.975	72.327	11.190	1.00	31.25	B_13
ATOM	3003	N	GLY	164	40.819	72.975	9.219	1.00	29.43	B_13
ATOM	3005	CA	GLY	164	40.291	74.324	9.340	1.00	30.64	B_13

```
ATOM   3006  C    GLY   164      41.402  75.344   9.424  1.00 30.89      B_13
ATOM   3007  O    GLY   164      41.101  76.564   9.368  1.00 26.89      B_13
ATOM   3008  OT   GLY   164      42.570  74.911   9.560  1.00 27.71      B_13
ATOM   3013  ZN   ZN    166      51.961  60.891  -2.865  1.00 28.31      BION
ATOM   3014  ZN   ZN    167      56.468  50.981   3.458  1.00 26.20      BION
ATOM   3015 CA   CA     168      63.096  53.752  -5.445  1.00 14.89      BION
ATOM   3016 CA   CA     165      50.705  55.618  13.085  1.00 15.79      BION
ATOM   3047  C5   WAY   169      54.585  56.119  -6.288  1.00 40.09      B693
ATOM   3048  CF1  WAY   169      54.019  54.934  -5.802  1.00 21.52      B693
ATOM   3049  CH   WAY   169      53.271  54.923  -4.624  1.00 32.32      B693
ATOM   3050  C2   WAY   169      53.100  56.104  -3.898  1.00 21.39      B693
ATOM   3051  C3   WAY   169      53.667  57.286  -4.369  1.00 18.26      B693
ATOM   3052  C4   WAY   169      54.402  57.308  -5.540  1.00 20.63      B693
ATOM   3053  N20  WAY   169      54.933  58.531  -5.964  1.00 22.15      B693
ATOM   3054  CD   WAY   169      54.297  59.340  -7.031  1.00 30.92      B693
ATOM   3055  C23  WAY   169      53.576  58.491  -8.087  1.00 20.75      B693
ATOM   3056  C28  WAY   169      54.224  58.114  -9.279  1.00 34.14      B693
ATOM   3057  C27  WAY   169      53.539  57.335 -10.228  1.00 33.99      B693
ATOM   3058  CM   WAY   169      52.209  56.944  -9.968  1.00 23.49      B693
ATOM   3059  N25  WAY   169      51.602  57.318  -8.814  1.00 23.61      B693
ATOM   3060  C24  WAY   169      52.246  58.071  -7.880  1.00 20.52      B693
ATOM   3061  S21  WAY   169      56.531  58.783  -5.660  1.00 20.46      B693
ATOM   3062  C16  WAY   169      56.457  60.446  -5.010  1.00 39.00      B693
ATOM   3063  C21  WAY   169      56.700  60.669  -3.634  1.00 28.79      B693
ATOM   3064  C20  WAY   169      56.656  61.967  -3.109  1.00 12.65      B693
ATOM   3065  C19  WAY   169      56.373  63.058  -3.946  1.00 15.68      B693
ATOM   3066  C18  WAY   169      56.126  62.828  -5.319  1.00 12.08      B693
ATOM   3067  C17  WAY   169      56.169  61.538  -5.852  1.00 15.19      B693
ATOM   3068  O33  WAY   169      56.337  64.360  -3.424  1.00 16.79      B693
ATOM   3069  C36  WAY   169      56.982  65.456  -4.084  1.00 20.80      B693
ATOM   3070  O15  WAY   169      56.973  57.923  -4.580  1.00 21.90      B693
ATOM   3071  O14  WAY   169      57.259  58.799  -6.913  1.00 10.86      B693
ATOM   3072  C7   WAY   169      53.486  58.556  -3.613  1.00 10.00      B693
ATOM   3073  N9   WAY   169      53.741  58.606  -2.303  1.00 10.00      B693
ATOM   3074  O10  WAY   169      53.539  59.846  -1.659  1.00 23.73      B693
ATOM   3075  O8   WAY   169      53.107  59.569  -4.154  1.00 15.89      B693
ATOM   3076  C29  WAY   169      55.383  55.968  -7.606  1.00 28.30      B693
ATOM      1  OH2  WAT   301      67.399  53.332  19.612  1.00 10.00      SOLV
ATOM      2  OH2  WAT   302      61.288  46.506  17.898  1.00 10.00      SOLV
ATOM      3  OH2  WAT   303      79.538  50.433  20.115  1.00 10.00      SOLV
ATOM      4  OH2  WAT   304      80.982  25.236  19.076  1.00 26.37      SOLV
ATOM      5  OH2  WAT   305      82.461  30.767  19.346  1.00 13.02      SOLV
ATOM      6  OH2  WAT   306      67.759  41.912   4.887  1.00 17.30      SOLV
ATOM      7  OH2  WAT   307      60.785  41.727  10.585  1.00 20.42      SOLV
ATOM      8  OH2  WAT   308      89.638  33.523  25.640  1.00 33.45      SOLV
ATOM      9  OH2  WAT   309      77.721  51.975   4.391  1.00 13.91      SOLV
ATOM     10  OH2  WAT   310      96.022  34.702   6.692  1.00 25.50      SOLV
ATOM     11  OH2  WAT   311      71.292  38.746  26.741  1.00 13.06      SOLV
ATOM     12  OH2  WAT   312      85.939  49.781   3.498  1.00 12.04      SOLV
ATOM     13  OH2  WAT   313      58.101  41.127  10.261  1.00 40.97      SOLV
ATOM     14  OH2  WAT   314      86.373  42.692   0.747  1.00 17.24      SOLV
ATOM     15  OH2  WAT   315      78.257  39.885  24.626  1.00 18.57      SOLV
ATOM     16  OH2  WAT   316      68.341  48.572  25.558  1.00 18.33      SOLV
ATOM     17  OH2  WAT   317      79.806  29.147  18.371  1.00 10.00      SOLV
ATOM     18  OH2  WAT   318      87.119  44.480  23.137  1.00 46.31      SOLV
ATOM     19  OH2  WAT   319      55.885  39.688  11.459  1.00 21.26      SOLV
ATOM     20  OH2  WAT   320      73.250  41.084   0.386  1.00 18.49      SOLV
ATOM     21  OH2  WAT   321      72.079  46.488  -6.835  1.00 27.48      SOLV
ATOM     22  OH2  WAT   322      71.923  37.638  -3.750  1.00 29.19      SOLV
ATOM     23  OH2  WAT   323      74.998  28.451   2.684  1.00 34.60      SOLV
ATOM     24  OH2  WAT   324      87.769  44.123   9.214  1.00 15.60      SOLV
ATOM     25  OH2  WAT   325      86.113  24.382  16.709  1.00 25.17      SOLV
ATOM     26  OH2  WAT   326      81.205  57.603   0.529  1.00 34.27      SOLV
ATOM     27  OH2  WAT   327      75.163  62.739  12.391  1.00 16.47      SOLV
ATOM     28  OH2  WAT   328      65.604  44.690   2.830  1.00 26.64      SOLV
ATOM     29  OH2  WAT   329      61.899  45.512  29.269  1.00 15.82      SOLV
ATOM     30  OH2  WAT   330      58.763  41.730   8.338  1.00 27.95      SOLV
ATOM     31  OH2  WAT   331      69.823  44.729   6.258  1.00 13.37      SOLV
ATOM     32  OH2  WAT   332      79.220  61.263  12.781  1.00 28.84      SOLV
ATOM     33  OH2  WAT   333      78.105  37.095  27.911  1.00 34.48      SOLV
ATOM     34  OH2  WAT   334      75.939  25.608  12.364  1.00 35.21      SOLV
ATOM     35  OH2  WAT   335      90.256  42.668  16.539  1.00 45.05      SOLV
ATOM     36  OH2  WAT   336      86.761  51.457  13.881  1.00 25.26      SOLV
ATOM     37  OH2  WAT   337      67.479  42.004  -5.009  1.00 33.30      SOLV
ATOM     38  OH2  WAT   338      82.018  50.963   8.823  1.00 19.80      SOLV
ATOM     39  OH2  WAT   339      80.278  32.895  -1.126  1.00 30.16      SOLV
ATOM     40  OH2  WAT   340      71.683  50.944  31.567  1.00 29.62      SOLV
```

ATOM	41	OH2	WAT	341	61.633	49.360	10.951	1.00	15.47	SOLV
ATOM	42	OH2	WAT	342	89.589	43.811	5.959	1.00	18.08	SOLV
ATOM	43	OH2	WAT	343	70.742	35.952	14.932	1.00	34.03	SOLV
ATOM	44	OH2	WAT	344	89.836	28.590	26.657	1.00	18.11	SOLV
ATOM	45	OH2	WAT	345	70.822	32.764	1.461	1.00	22.35	SOLV
ATOM	46	OH2	WAT	346	63.056	34.653	0.491	1.00	29.51	SOLV
ATOM	47	OH2	WAT	347	58.054	46.282	2.363	1.00	10.00	SOLV
ATOM	48	OH2	WAT	348	67.914	58.660	-6.267	1.00	18.30	SOLV
ATOM	49	OH2	WAT	349	70.170	56.725	0.575	1.00	11.89	SOLV
ATOM	50	OH2	WAT	350	55.922	73.897	0.623	1.00	18.86	SOLV
ATOM	51	OH2	WAT	351	73.489	53.195	2.061	1.00	24.35	SOLV
ATOM	52	OH2	WAT	352	58.033	50.530	19.075	1.00	25.52	SOLV
ATOM	53	OH2	WAT	353	63.245	57.302	17.340	1.00	13.88	SOLV
ATOM	54	OH2	WAT	354	58.442	71.334	-5.670	1.00	17.51	SOLV
ATOM	55	OH2	WAT	355	62.535	61.154	16.706	1.00	12.38	SOLV
ATOM	56	OH2	WAT	356	66.949	51.163	-10.284	1.00	17.92	SOLV
ATOM	57	OH2	WAT	357	57.588	54.191	9.850	1.00	17.88	SOLV
ATOM	58	OH2	WAT	358	64.836	48.085	4.627	1.00	17.80	SOLV
ATOM	59	OH2	WAT	359	66.445	61.785	19.640	1.00	24.12	SOLV
ATOM	60	OH2	WAT	360	55.740	42.557	0.533	1.00	27.32	SOLV
ATOM	61	OH2	WAT	361	74.075	57.146	13.179	1.00	18.01	SOLV
ATOM	62	OH2	WAT	362	46.987	69.315	-2.545	1.00	11.87	SOLV
ATOM	63	OH2	WAT	363	53.842	52.266	-2.612	1.00	25.20	SOLV
ATOM	64	OH2	WAT	364	33.425	65.313	-4.686	1.00	28.97	SOLV
ATOM	65	OH2	WAT	365	45.633	51.173	10.502	1.00	31.97	SOLV
ATOM	66	OH2	WAT	366	39.040	71.050	-0.722	1.00	20.81	SOLV
ATOM	67	OH2	WAT	367	54.517	67.335	-6.251	1.00	46.24	SOLV
ATOM	68	OH2	WAT	368	45.083	67.138	20.314	1.00	29.47	SOLV
ATOM	69	OH2	WAT	369	65.758	67.669	-6.655	1.00	14.69	SOLV
ATOM	70	OH2	WAT	370	44.943	78.174	12.948	1.00	23.88	SOLV
ATOM	71	OH2	WAT	371	37.141	57.403	1.723	1.00	23.72	SOLV
ATOM	72	OH2	WAT	372	62.407	66.806	13.368	1.00	13.36	SOLV
ATOM	73	OH2	WAT	373	50.776	47.263	5.661	1.00	38.22	SOLV
ATOM	74	OH2	WAT	374	56.697	47.264	11.752	1.00	24.75	SOLV
ATOM	75	OH2	WAT	375	42.566	60.884	15.739	1.00	16.25	SOLV
ATOM	76	OH2	WAT	376	59.299	74.342	13.838	1.00	31.27	SOLV
ATOM	77	OH2	WAT	377	72.976	63.691	-0.667	1.00	20.36	SOLV
ATOM	78	OH2	WAT	378	72.876	60.516	-6.752	1.00	34.24	SOLV
ATOM	79	OH2	WAT	379	63.998	68.760	16.371	1.00	19.04	SOLV
ATOM	80	OH2	WAT	380	44.947	66.728	-2.566	1.00	29.51	SOLV
ATOM	81	OH2	WAT	381	57.690	61.926	-9.414	1.00	29.01	SOLV
ATOM	82	OH2	WAT	382	44.595	80.810	5.831	1.00	27.43	SOLV
ATOM	83	OH2	WAT	383	78.065	36.583	24.121	1.00	14.08	SOLV
ATOM	84	OH2	WAT	384	42.289	64.651	-0.868	1.00	25.57	SOLV
ATOM	85	OH2	WAT	385	59.851	68.458	-12.381	1.00	30.18	SOLV
ATOM	86	OH2	WAT	386	53.784	72.644	-4.782	1.00	22.35	SOLV
ATOM	87	OH2	WAT	387	72.793	27.922	8.925	1.00	32.13	SOLV
ATOM	88	OH2	WAT	388	57.224	68.062	-6.072	1.00	17.87	SOLV
ATOM	89	OH2	WAT	389	45.210	44.988	4.285	1.00	25.10	SOLV
ATOM	90	OH2	WAT	390	49.413	53.782	1.546	1.00	21.68	SOLV
ATOM	91	OH2	WAT	391	45.232	59.677	1.393	1.00	19.25	SOLV
ATOM	92	OH2	WAT	392	42.551	59.954	5.056	1.00	27.30	SOLV
ATOM	93	OH2	WAT	393	58.412	43.750	3.948	1.00	58.70	SOLV
ATOM	94	OH2	WAT	394	56.942	54.199	-2.588	1.00	31.14	SOLV
ATOM	95	OH2	WAT	395	55.216	51.994	9.824	1.00	13.25	SOLV
ATOM	96	OH2	WAT	396	51.642	54.651	14.874	1.00	10.00	SOLV
ATOM	97	OH2	WAT	397	48.690	56.156	13.991	1.00	28.59	SOLV
ATOM	98	OH2	WAT	398	74.412	37.913	0.396	1.00	12.55	SOLV
ATOM	99	OH2	WAT	399	81.920	53.968	18.267	1.00	14.05	SOLV
ATOM	100	OH2	WAT	400	70.413	41.780	1.170	1.00	16.68	SOLV
ATOM	101	OH2	WAT	401	71.098	53.544	2.407	1.00	27.63	SOLV
ATOM	102	OH2	WAT	402	94.383	32.979	9.497	1.00	27.97	SOLV
ATOM	103	OH2	WAT	403	70.765	66.069	16.389	1.00	38.09	SOLV
ATOM	104	OH2	WAT	404	78.651	34.890	29.495	1.00	48.60	SOLV
ATOM	105	OH2	WAT	405	80.289	39.811	24.727	1.00	20.74	SOLV
ATOM	106	OH2	WAT	406	63.627	47.414	7.301	1.00	40.21	SOLV
ATOM	107	OH2	WAT	407	74.679	30.772	11.524	1.00	37.03	SOLV
ATOM	108	OH2	WAT	408	80.240	36.041	26.681	1.00	27.42	SOLV
ATOM	109	OH2	WAT	409	84.971	25.909	18.426	1.00	24.96	SOLV
ATOM	110	OH2	WAT	410	57.832	41.294	5.792	1.00	71.90	SOLV
ATOM	111	OH2	WAT	411	55.484	68.139	-9.086	1.00	48.47	SOLV
ATOM	112	OH2	WAT	412	65.535	68.260	2.400	1.00	26.24	SOLV
ATOM	113	OH2	WAT	413	80.085	42.291	-3.144	1.00	26.49	SOLV
ATOM	114	OH2	WAT	414	82.088	37.456	27.733	1.00	42.54	SOLV
ATOM	115	OH2	WAT	415	61.020	53.195	21.566	1.00	38.16	SOLV
ATOM	116	OH2	WAT	416	55.968	70.365	-5.096	1.00	28.42	SOLV
ATOM	117	OH2	WAT	417	51.619	57.620	-0.487	1.00	41.81	SOLV

```
ATOM    118  OH2 WAT   418      40.651  66.108   2.086  1.00 40.11      SOLV
ATOM    119  OH2 WAT   419      58.453  49.818   7.926  1.00 38.96      SOLV
ATOM    120  OH2 WAT   420      53.768  51.716  13.623  1.00 43.62      SOLV
ATOM    121  OH2 WAT   421      76.068  60.373  21.292  1.00 39.30      SOLV
ATOM    122  OH2 WAT   422      56.186  50.034  17.422  1.00 37.47      SOLV
END
```

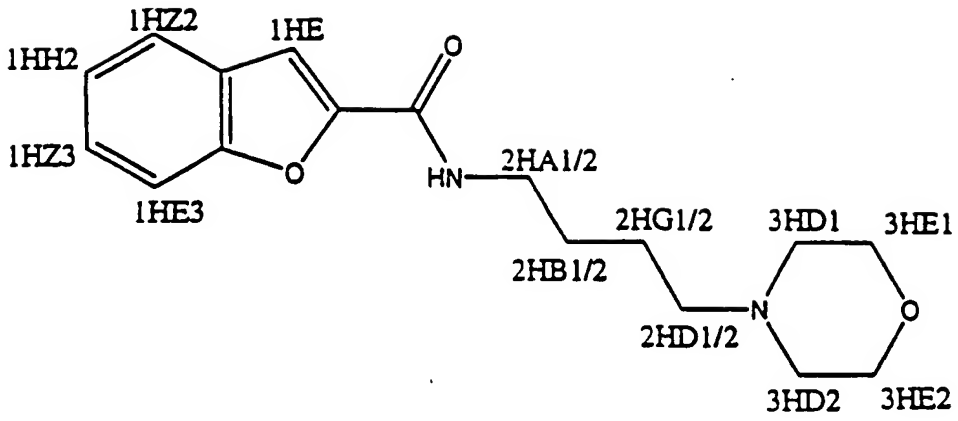
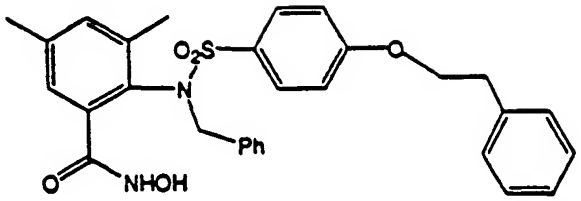

1HZ2
1HE
1HH2
O
1HZ3
O
HN
2HA1/2
1HE3
2HG1/2
3HD1
3HE1
2HB1/2
N
O
2HD1/2
3HD2
3HE2

FIG. 6

Compound C



Compound D

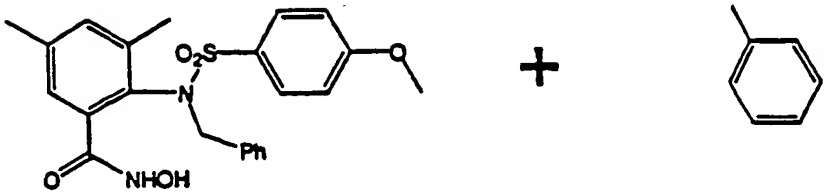


FIG. 7

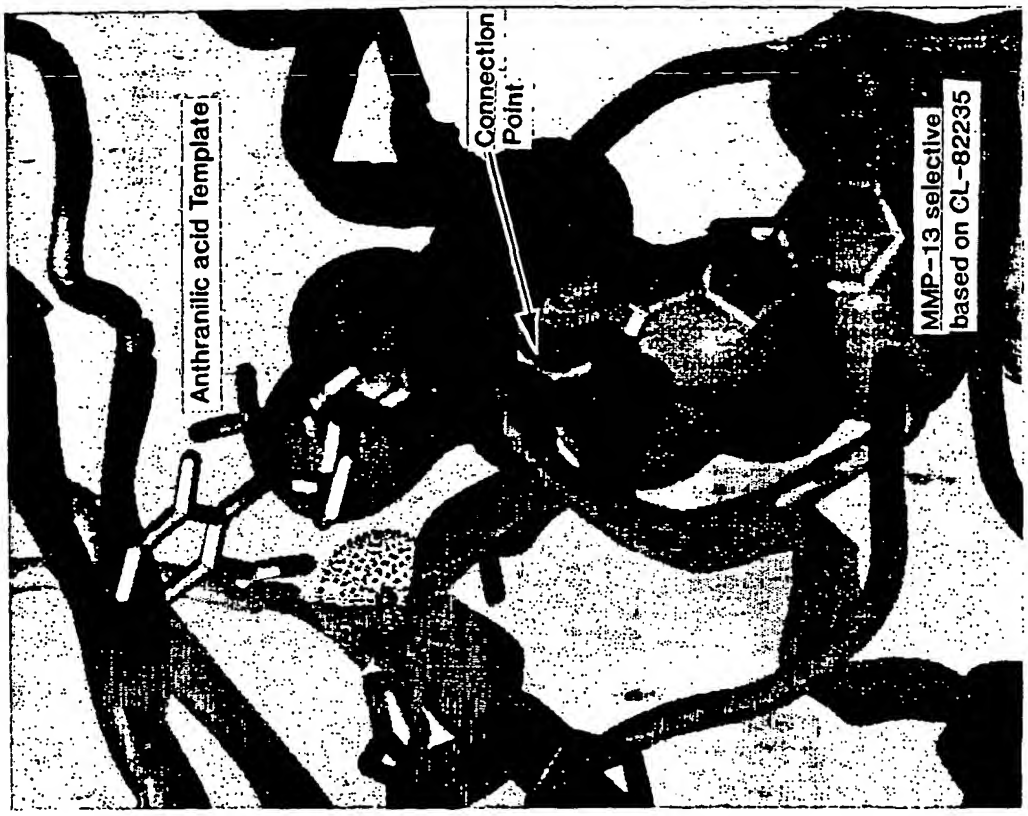
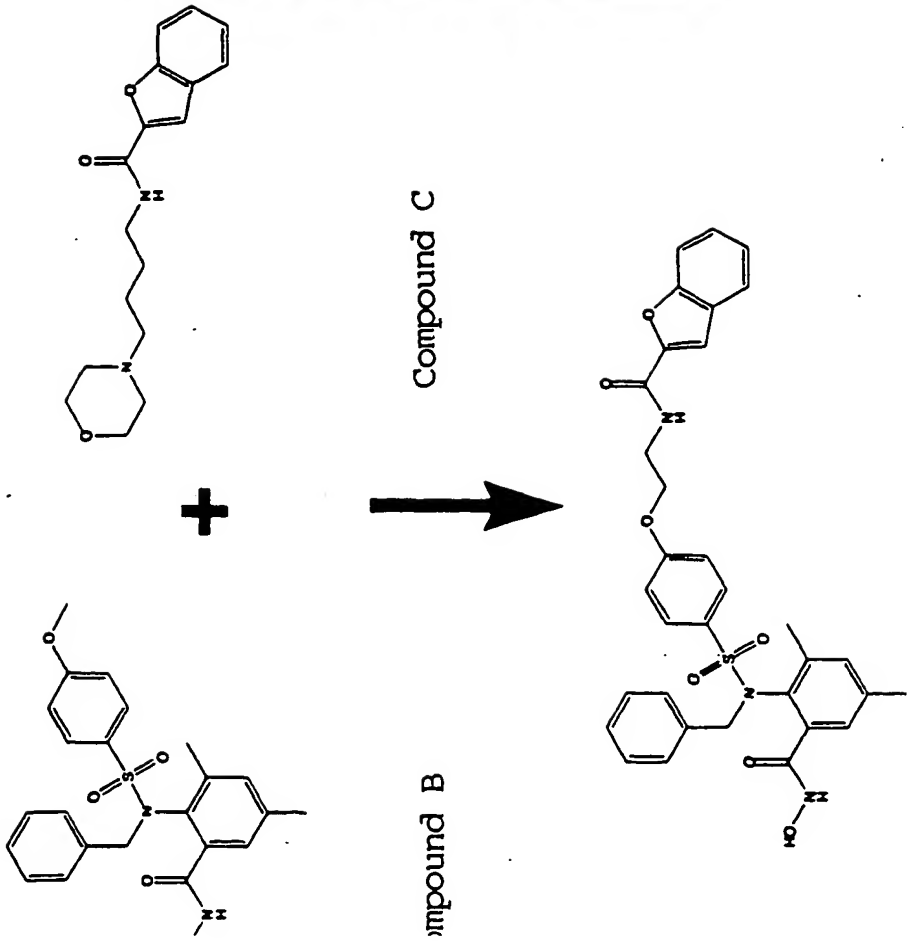

Anthranilic acid Template
Connection Point
MMP-13 selective based on CL-82235

FIG. 8


Compound C
Compound E

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US01/05150

A. *CLASSIFICATION OF SUBJECT MATTER

IPC(7) :G01N 9/00, 33/48
US CL :435/183; 702/22

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 435/183; 702/22

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

NONE

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

STN: WEST

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	GOMIS-RUTH, F.X. et al. The helping hand of collagenase-3 (MMP-13: 2.7, ANG> crystal structure of its C-terminal haemopexin-like domain. Journal Mol. Biol. 1996, Vol. 264, No. 3, pages 556-566, see entire document.	8-14
X	US 6,008,243 A (BENDER et al.) 28 December 1999(28.12.99), see entire document.	1-7, 15-20

☐ Further documents are listed in the continuation of Box C. ☐ See patent family annex.

*	Special categories of cited documents:	"T"	later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"A"	document defining the general state of the art which is not considered to be of particular relevance	"X"	document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"E"	earlier document published on or after the international filing date	"Y"	document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"L"	document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	"&"	document member of the same patent family
"O"	document referring to an oral disclosure, use, exhibition or other means		
"P"	document published prior to the international filing date but later than the priority date claimed		

Date of the actual completion of the international search 12 JULY 2001	Date of mailing of the international search report 30 JUL 2001
Name and mailing address of the ISA/US Commissioner of Patents and Trademarks Box PCT Washington, D.C. 20231 Facsimile No. (703) 305-3230	Authorized officer Kathleen Lawrence for AMY J. HARTTER Telephone No. (703) 308-0196

Form PCT/ISA/210 (second sheet) (July 1998) *

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US01/05150

Box I Observations where certain claims were found unsearchable (Continuation of item 1 of first sheet)

This international report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☐ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box II Observations where unity of invention is lacking (Continuation of item 2 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

Please See Extra Sheet.

1. ☒ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.

2. ☐ As all searchable claims could be searched without effort justifying an additional fee, this Authority did not invite payment of any additional fee.

3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:

4. ☐ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:

Remark on Protest

☐ The additional search fees were accompanied by the applicant's protest.

☐ No protest accompanied the payment of additional search fees.

BOX II. OBSERVATIONS WHERE UNITY OF INVENTION WAS LACKING
This ISA found multiple inventions as follows:

This application contains the following inventions or groups of inventions which are not so linked as to form a single inventive concept under PCT Rule 13.1. In order for as inventions to searched the appropriate search fees must be paid.
Group I which consists of claims 1-7 is distinct as it addresses itself to the solution complex of the mixture of MMP-13 and the defined "Compound A." The solution is clearly distinct and different from the crystal complex, active site and methods that are claimed in succeeding groups and according claims.

Group II consists of claims 8-14. These claims pertain to the actual product of the crystal complexion its entirety. Thus it is distinct from Groups I and Groups 3-4. The group claims the whole crystal known as "Compound A". and the crystal is not in any other type of alternate environment or with any additional accoutrements.

Group III encompasses the claims of 15-20. These claims consist of the active site of the molecule of MMP-13. This chemical is a portion of the solution claimed in the first group and thus separate and distinct from the solution of Group I or the separate entity of "Compound A" that is claimed in Group 2. Thus these Groups are separate.

Group IV consists of claims 21-32 which claim a method of identifying an inhibitor or activator of the MMP-13 compound. The method that is embodied within this Group is clearly different from the proceeding groups. Firstly the claims within Group 4 are directed toward a method of accomplishing the task of identifying different entities and not a product itself. Secondly its actions are addressed to entities outside the compound itself and not limited to "Compound A" of the MMP-13. Based on the aforementioned reasons and the distinct nature of the claims defined in each of the groups, the instant application has a lack of unity due to each group having a different Special Technical Feature a summarized above for each group.